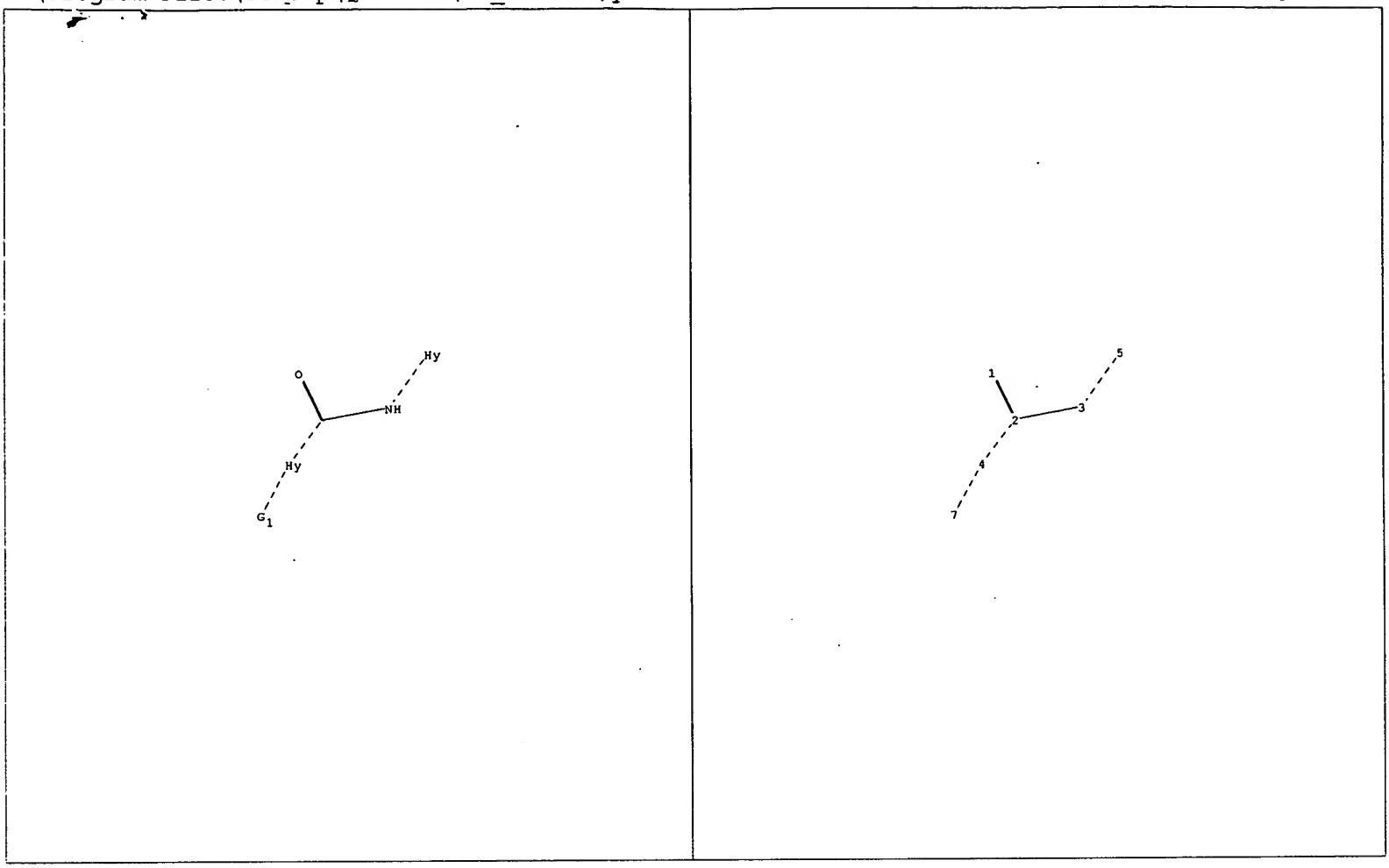
C:\Program Files\Stnexp\Queries\10_532847\qaz-a.str

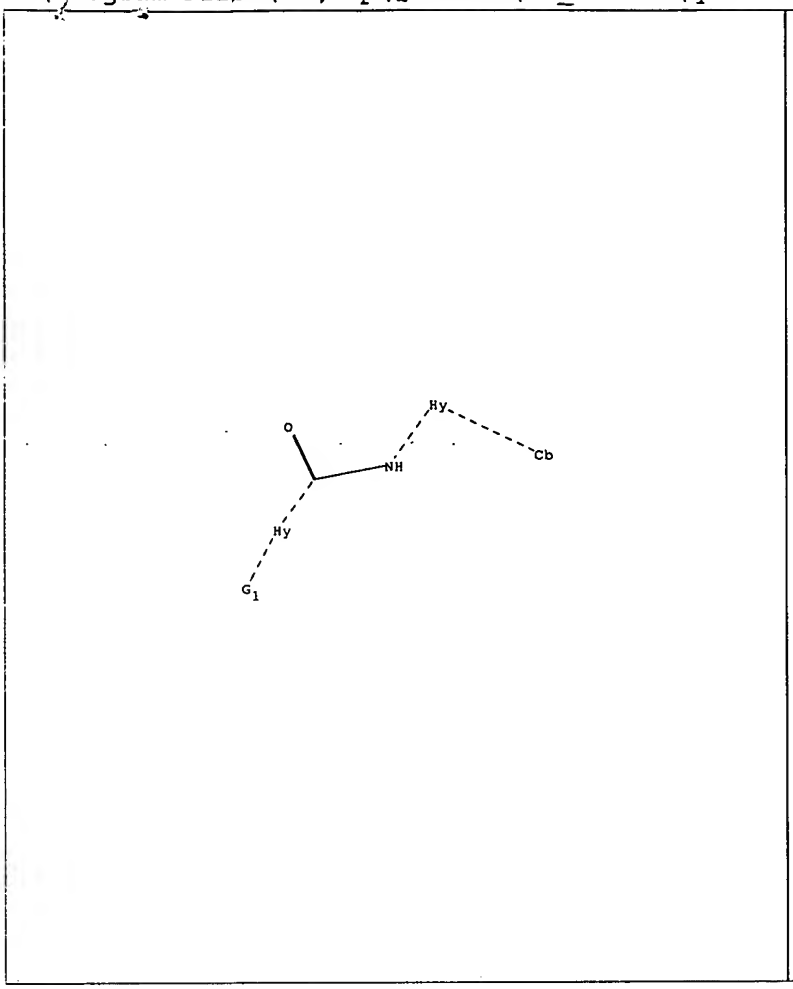
structure "L1"

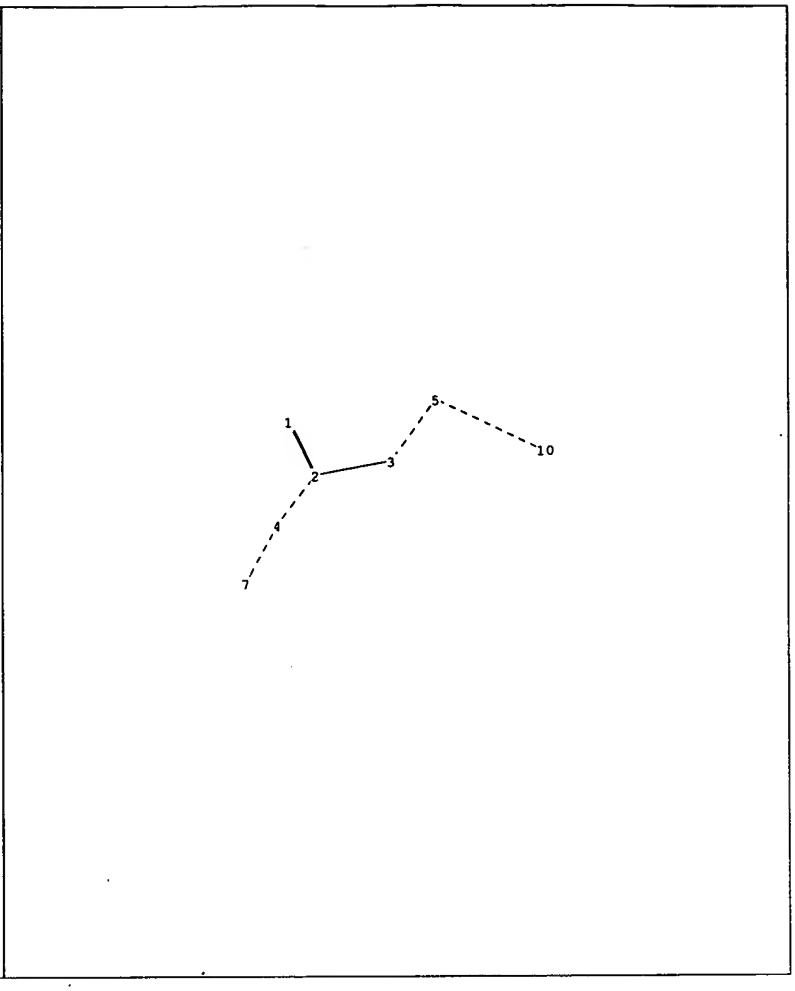



```
chain nodes :
    1  2  3  4  5  7
chain bonds :
    1-2  2-3  2-4  3-5  4-7
exact/norm bonds :
    1-2  2-3  2-4  3-5  4-7


G1:CN,NO2,X,Ak

Match level :
    1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  7:CLASS
Generic attributes :
    4:
    Number of Carbon Atoms : less than 7
    Type of Ring System    : Monocyclic
    5:
    Saturation             : Unsaturated
    Number of Carbon Atoms : less than 7
    Number of Hetero Atoms : Exactly 1
    Type of Ring System    : Monocyclic

Element Count :
    Node 5: Limited
        S,S1
        C,C4
        O,O0
```

C:\Program Files\Stnexp\Queries\10_532847\qaz-b.str

structure "L6"





chain nodes :
1 2 3 4 5 7 10
chain bonds :
1-2 2-3 2-4 3-5 4-7 5-10
exact/norm bonds :
1-2 2-3 2-4 3-5 4-7 5-10

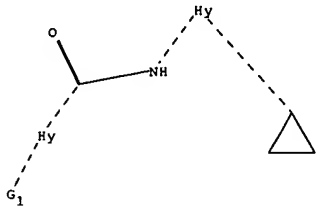
G1:CN,NO2,X,Ak

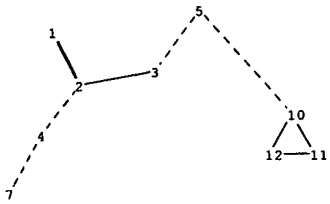
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:CLASS 10:Atom
Generic attributes :
4:
Number of Carbon Atoms : less than 7
Type of Ring System : Monocyclic
5:
Saturation : Unsaturated
Number of Carbon Atoms : less than 7
Number of Hetero Atoms : Exactly 1
Type of Ring System : Monocyclic

Element Count :
Node 5: Limited
S,S1
C,C4
O,O0

C:\Program Files\Stnexp\Queries\10_532847\qaz-c.str

Structure "L 8"





chain nodes :
1 2 3 4 5 7
ring nodes :
10 11 12
chain bonds :
1-2 2-3 2-4 3-5 4-7 5-10
ring bonds :
10-11 10-12 11-12
exact/norm bonds :
1-2 2-3 2-4 3-5 4-7 5-10 10-11 10-12 11-12

G1:CN,NO2,X,Ak

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:CLASS 10:Atom 11:Atom 12:Atom
Generic attributes :
4:
Number of Carbon Atoms : less than 7
Type of Ring System : Monocyclic
5:
Saturation : Unsaturated
Number of Carbon Atoms : less than 7
Number of Hetero Atoms : Exactly 1
Type of Ring System : Monocyclic

Element Count :

Node 5: Limited
S,S1
C,C4
O,O0
N,N0

Search history - Part A


```
=> d his full

     (FILE 'HOME' ENTERED AT 14:36:35 ON 21 MAR 2006)

     FILE 'REGISTRY' ENTERED AT 14:36:43 ON 21 MAR 2006
L1             STRUCTURE UPLOADED
L2               0 SEA SSS SAM L1
L3          546562 SEA ABB=ON  PLU=ON  SC4/ES
L4               9 SEA SUB=L3 SSS SAM L1
L5            2304 SEA SUB=L3 SSS FUL L1
                   SAVE TEMP L5 QAZ847STRA/A

     FILE 'STNGUIDE' ENTERED AT 14:40:17 ON 21 MAR 2006

     FILE 'REGISTRY' ENTERED AT 14:42:06 ON 21 MAR 2006
L6             STRUCTURE UPLOADED
L7              43 SEA SUB=L5 SSS SAM L6

     FILE 'STNGUIDE' ENTERED AT 14:44:07 ON 21 MAR 2006

     FILE 'REGISTRY' ENTERED AT 14:44:40 ON 21 MAR 2006
L8             STRUCTURE UPLOADED
L9              29 SEA SUB=L5 SSS SAM L8
L10            630 SEA SUB=L5 SSS FUL L8
                   SAVE TEMP L10 QAZ847STRC/A

     FILE 'CAPLUS' ENTERED AT 14:46:29 ON 21 MAR 2006
L11             1 SEA ABB=ON  PLU=ON  L10

     FILE 'REGISTRY' ENTERED AT 14:47:08 ON 21 MAR 2006
L12            ANALYZE PLU=ON  L10 1- LC :        4 TERMS
               D

     FILE 'STNGUIDE' ENTERED AT 14:47:48 ON 21 MAR 2006

     FILE 'CAPLUS' ENTERED AT 14:48:00 ON 21 MAR 2006
L13           134 SEA ABB=ON  PLU=ON  L5
                   S L6

     FILE 'REGISTRY' ENTERED AT 14:50:48 ON 21 MAR 2006
L*** DEL       43 S L6 SSS SAM SUB=L5

     FILE 'CAPLUS' ENTERED AT 14:50:49 ON 21 MAR 2006
L*** DEL        5 S L14 SSS SUBSET=L5 SAM
                   D COST

     FILE 'REGISTRY' ENTERED AT 14:51:43 ON 21 MAR 2006
L14             43 SEA SUB=L5 SSS SAM L6
L15           1135 SEA SUB=L5 SSS FUL L6
                   SAVE TEMP QAZ847STRB/A L15

     FILE 'CAPLUS' ENTERED AT 14:52:41 ON 21 MAR 2006
L16             23 SEA ABB=ON  PLU=ON  L15

     FILE 'REGISTRY' ENTERED AT 14:53:39 ON 21 MAR 2006
L17            505 SEA ABB=ON  PLU=ON  L15 NOT L10

     FILE 'CAPLUS' ENTERED AT 14:54:02 ON 21 MAR 2006
L18             22 SEA ABB=ON  PLU=ON  L17
```

```
     FILE 'BEILSTEIN' ENTERED AT 14:56:39 ON 21 MAR 2006
L19            0 SEA SSS SAM L8

     FILE 'MARPAT' ENTERED AT 14:57:37 ON 21 MAR 2006
L20            0 SEA SSS SAM L8
L21            6 SEA SSS FUL L8
L22            5 SEA ABB=ON  PLU=ON  L21/COM

     FILE 'CHEMCATS' ENTERED AT 15:00:33 ON 21 MAR 2006
L23            2 SEA ABB=ON  PLU=ON  L10

     FILE 'STNGUIDE' ENTERED AT 15:01:06 ON 21 MAR 2006

     FILE 'CHEMCATS' ENTERED AT 15:01:25 ON 21 MAR 2006

     FILE 'STNGUIDE' ENTERED AT 15:01:52 ON 21 MAR 2006

     FILE 'CAPLUS' ENTERED AT 15:06:43 ON 21 MAR 2006
L24           85 SEA ABB=ON  PLU=ON  EHRENFREUND J?/AU
L25          143 SEA ABB=ON  PLU=ON  TOBLER H?/AU
L26         1251 SEA ABB=ON  PLU=ON  WALTER H?/AU
L27           12 SEA ABB=ON  PLU=ON  (L24 AND (L25 OR L26)) OR (L25 AND L26)
L28            1 SEA ABB=ON  PLU=ON  L27 AND L11

     FILE 'REGISTRY' ENTERED AT 15:09:32 ON 21 MAR 2006
                D STAT QUE L10
                D STAT QUE L15

     FILE 'CAPLUS' ENTERED AT 15:14:21 ON 21 MAR 2006
                D STAT QUE L27
                D IBIB ABS HITIND L27 1-12

     FILE 'CAPLUS' ENTERED AT 15:16:26 ON 21 MAR 2006
                D QUE NOS L11
                D L12

     FILE 'CHEMCATS' ENTERED AT 15:17:21 ON 21 MAR 2006
                D QUE NOS L23
                D IALL L23 1-2

     FILE 'MARPAT' ENTERED AT 15:18:39 ON 21 MAR 2006
                D STAT QUE L22

     FILE 'CAPLUS, MARPAT' ENTERED AT 15:19:24 ON 21 MAR 2006
L29            5 DUP REM L11 L22 (1 DUPLICATE REMOVED)
                     ANSWER '1' FROM FILE CAPLUS
                     ANSWERS '2-5' FROM FILE MARPAT
                D IBIB ABS L29 1
                D IBIB ABS HIT L29 2-5

     FILE 'CAPLUS' ENTERED AT 15:21:34 ON 21 MAR 2006
                D QUE NOS L18
                D IBIB ABS HITSTR L18 1-22


     FILE HOME

     FILE REGISTRY
     Property values tagged with IC are from the ZIC/VINITI data file
     provided by InfoChem.
```

STRUCTURE FILE UPDATES: 20 MAR 2006 HIGHEST RN 877371-73-8
DICTIONARY FILE UPDATES: 20 MAR 2006 HIGHEST RN 877371-73-8

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

****
*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*
****

Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

FILE STNGUIDE
FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Mar 17, 2006 (20060317/UP).

FILE CAPLUS

FILE COVERS 1907 - 21 Mar 2006 VOL 144 ISS 13
FILE LAST UPDATED: 20 Mar 2006 (20060320/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/infopolicy.html

FILE BEILSTEIN
FILE LAST UPDATED ON MARCH 15, 2006

FILE COVERS 1771 TO 2006.
FILE CONTAINS 9,516,393 SUBSTANCES

>>>PLEASE NOTE: Reaction Data and substance data are stored in separate documents and can not be searched together in one query. Reaction data for BEILSTEIN compounds may be displayed immediately with the display codes PRE (preparations) and REA (reactions). A substance answer set retrieved after the search for a chemical name, a compounds with available reaction information by combining with PRE/FA, REA/FA or more generally with RX/FA. The BEILSTEIN Registry Number (BRN) is the link between a BEILSTEIN compound and belonging reactions. For mo detailed reaction searches BRNs can be searched as reaction partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

****
* PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST. *
* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE *
* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE *
* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS. *
* FOR PRICE INFORMATION SEE HELP COST *
****

NEW

*** PATENT NUMBERS (PN) AND BABS ACCESSION NUMBERS (BABSAN) CAN NOW BE SEARCHED, SELECTED AND TRANSFERRED.**

*** NEW DISPLAY FORMATS ALLREF, ALLP AND BABSAN SHOW ALL REFERENCES, ALL PATENT REFERENCES, OR ALL BABS ACCESSION NUMBERS FOR A COMPOUND AT A GLANCE.**

FILE MARPAT
FILE CONTENT: 1961-PRESENT VOL 144 ISS 12 (20060317/ED)

SOME MARPAT RECORDS ARE DERIVED FROM INPI DATA FOR 1961-1987

MOST RECENT CITATIONS FOR PATENTS FROM MAJOR ISSUING AGENCIES
(COVERAGE TO THESE DATES IS NOT COMPLETE):

US 2006035965 16 FEB 2006
DE 102004030305 12 JAN 2006
EP 1614691 11 JAN 2006
JP 2006008639 12 JAN 2006
WO 2006012333 02 FEB 2006
GB 2415429 28 DEC 2005
FR 2873371 27 JAN 2006
RU 2267521 10 JAN 2006
CA 2472818 30 DEC 2005

Expanded G-group definition display now available.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

FILE CHEMCATS

FILE LAST UPDATED 18 MARCH 2006 (20060318/UP)

For details on recent updates in CHEMCATS, enter NEWS FILE at an arrow prompt. For the list of suppliers currently in the file, enter HELP SPA, HELP SPBC, HELP SPDH, HELP SPIN, HELP SPOP, and HELP SPQZ. For the list of current catalogs, enter HELP CTA, HELP CTBC, HELP CTDH, HELP CTIN, HELP CTOP, and HELP CTQZ.

This database is provided on an "as is" basis. Please consult the suppliers for current information regarding pricing, regional availability, available quantities, purities, etc. THERE ARE NO WARRANTIES OF ANY KIND, EITHER EXPRESSED OR IMPLIED. ACS is not liable for any loss of profit, goodwill or any other damages arising out of the use of this database.

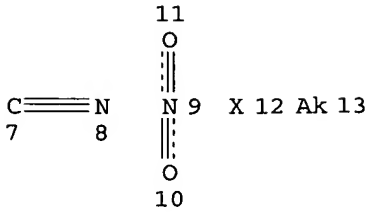
CHEMCATS now contains more than 8 million records. See HELP CONTENT and NEWS FILE for details.

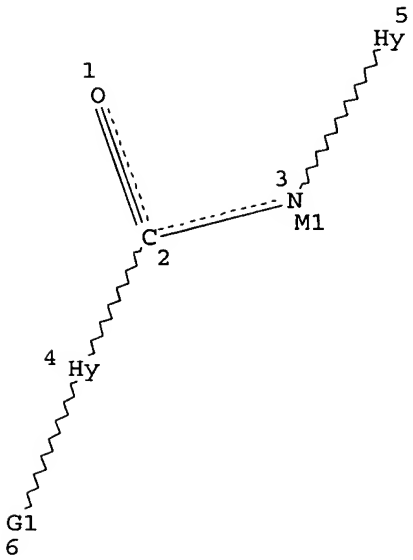
=>

PART A

STRUCTURE QUERIES

```
=> file registry
FILE 'REGISTRY' ENTERED AT 15:09:32 ON 21 MAR 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2006 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   20 MAR 2006  HIGHEST RN 877371-73-8
DICTIONARY FILE UPDATES:  20 MAR 2006  HIGHEST RN 877371-73-8

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

**********************************************************************
*                                                                    *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,   *
* effective March 20, 2005.  A new display format, IDERL, is now    *
* available and contains the CA role and document type information. *
*                                                                    *
**********************************************************************

Structure search iteration limits have been increased.  See HELP SLIMITS
for details.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=> d stat que L10
L1              STR
```

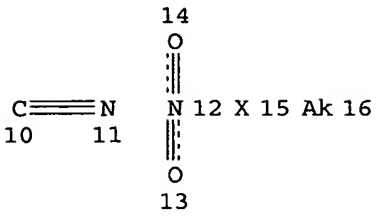


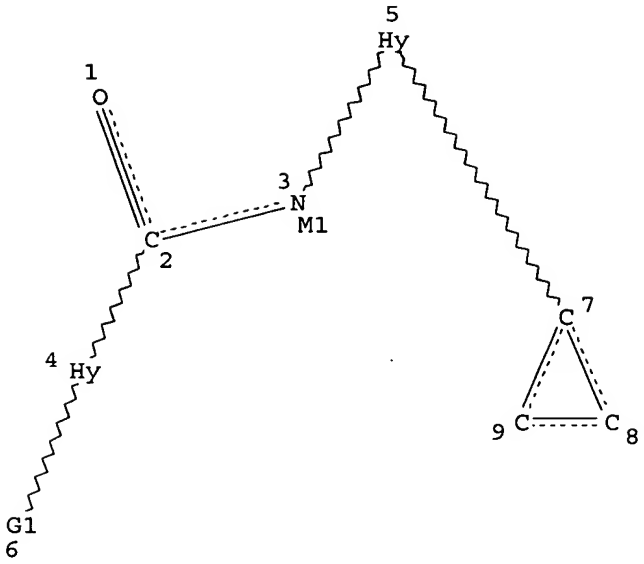


VAR G1=7/9/12/13
NODE ATTRIBUTES:
HCOUNT IS M1 AT 3
NSPEC IS C AT 1
NSPEC IS C AT 2
NSPEC IS C AT 3
NSPEC IS C AT 4
NSPEC IS C AT 5
NSPEC IS C AT 6
DEFAULT MLEVEL IS ATOM
MLEVEL IS CLASS AT 7 8 9 10 11 12 13
GGCAT IS MCY LOC AT 4
GGCAT IS MCY LOC LOQ UNS AT 5
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS E4 C E0 N E0 O E1 S AT 5

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE
L3 546562 SEA FILE=REGISTRY ABB=ON PLU=ON SC4/ES
L5 2304 SEA FILE=REGISTRY SUB=L3 SSS FUL L1
L8 STR





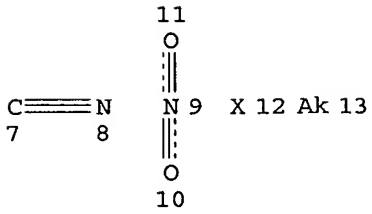
VAR G1=10/12/15/16
NODE ATTRIBUTES:
HCOUNT IS M1 AT 3
NSPEC IS C AT 1
NSPEC IS C AT 2
NSPEC IS C AT 3
NSPEC IS C AT 4
NSPEC IS C AT 5
NSPEC IS C AT 6
NSPEC IS R AT 7
NSPEC IS R AT 8
NSPEC IS R AT 9
DEFAULT MLEVEL IS ATOM
MLEVEL IS CLASS AT 10 11 12 13 14 15 16
GGCAT IS MCY LOC AT 4
GGCAT IS MCY LOC LOQ UNS AT 5
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS E4 C E0 N E0 O E1 S AT 5

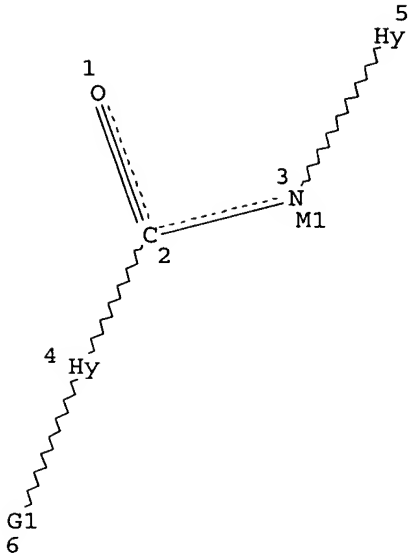
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 16

STEREO ATTRIBUTES: NONE
L10 630 SEA FILE=REGISTRY SUB=L5 SSS FUL L8 narrower structure hits

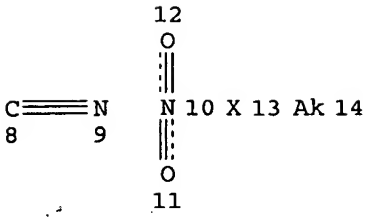
100.0% PROCESSED 2304 ITERATIONS 630 ANSWERS
SEARCH TIME: 00.00.01

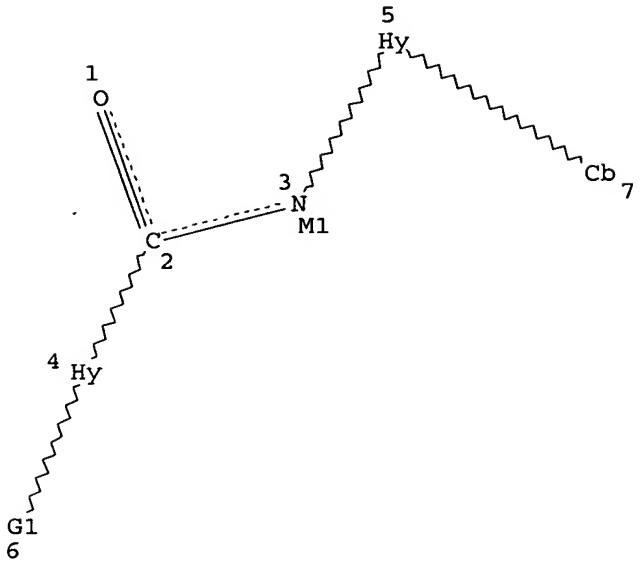
```
=> d stat que L15
L1              STR
```






```
VAR G1=7/9/12/13
NODE ATTRIBUTES:
HCOUNT  IS M1     AT   3
NSPEC   IS C      AT   1
NSPEC   IS C      AT   2
NSPEC   IS C      AT   3
NSPEC   IS C      AT   4
NSPEC   IS C      AT   5
NSPEC   IS C      AT   6
DEFAULT MLEVEL IS ATOM
MLEVEL  IS CLASS  AT   7  8  9 10 11 12 13
GGCAT   IS MCY  LOC  AT   4
GGCAT   IS MCY  LOC  LOQ  UNS  AT   5
DEFAULT ECLEVEL IS LIMITED
ECOUNT  IS E4 C  E0 N  E0 O  E1 S  AT   5

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  13

STEREO ATTRIBUTES: NONE
L3       546562 SEA FILE=REGISTRY ABB=ON  PLU=ON  SC4/ES
L5         2304 SEA FILE=REGISTRY SUB=L3 SSS FUL L1
L6              STR
```






```
VAR G1=8/10/13/14
NODE ATTRIBUTES:
HCOUNT  IS M1     AT   3
NSPEC   IS C      AT   1
NSPEC   IS C      AT   2
NSPEC   IS C      AT   3
NSPEC   IS C      AT   4
NSPEC   IS C      AT   5
NSPEC   IS C      AT   6
NSPEC   IS C      AT   7
DEFAULT MLEVEL IS ATOM
MLEVEL  IS CLASS  AT   8  9 10 11 12 13 14
GGCAT   IS MCY  LOC  AT   4
GGCAT   IS MCY  LOC  LOQ  UNS  AT   5
DEFAULT ECLEVEL IS LIMITED
ECOUNT  IS E4 C  E0 N  E0 O  E1 S  AT   5

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  14

STEREO ATTRIBUTES: NONE
L15        1135 SEA FILE=REGISTRY SUB=L5 SSS FUL L6

100.0% PROCESSED    2304 ITERATIONS                    1135 ANSWERS
SEARCH TIME: 00.00.01


=> file caplus
FILE 'CAPLUS' ENTERED AT 15:14:21 ON 21 MAR 2006
```

broader structure hits

AUTHOR SEARCH

FILE COVERS 1907 - 21 Mar 2006 VOL 144 ISS 13
FILE LAST UPDATED: 20 Mar 2006 (20060320/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

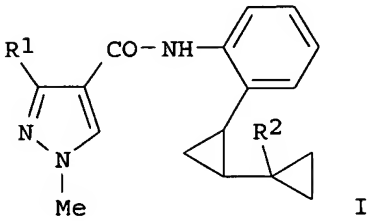
http://www.cas.org/infopolicy.html
'OBI' IS DEFAULT SEARCH FIELD FOR 'CAPLUS' FILE

```
=> d stat que L27
L24          85 SEA FILE=CAPLUS ABB=ON  PLU=ON  EHRENFREUND J?/AU
L25         143 SEA FILE=CAPLUS ABB=ON  PLU=ON  TOBLER H?/AU
L26        1251 SEA FILE=CAPLUS ABB=ON  PLU=ON  WALTER H?/AU
L27          12 SEA FILE=CAPLUS ABB=ON  PLU=ON  (L24 AND (L25 OR L26)) OR (L25
                AND L26)


=> d ibib abs hitind L27 1-12

L27  ANSWER 1 OF 12  CAPLUS  COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER:        2006:151202  CAPLUS
DOCUMENT NUMBER:         144:207363
TITLE:                   Synergistic fungicidal compositions comprising
                         pyrazole derivatives
INVENTOR(S):             Walter, Harald; Neuenschwander, Urs; Zeun,
                         Ronald; Ehrenfreund, Josef; Tobler,
                         Hans; Corsi, Camilla; Lamberth, Clemens
PATENT ASSIGNEE(S):      Syngenta Participations AG, Switz.
SOURCE:                  PCT Int. Appl., 104 pp.
                         CODEN: PIXXD2
DOCUMENT TYPE:           Patent
LANGUAGE:                English
FAMILY ACC. NUM. COUNT:  1
PATENT INFORMATION:

     PATENT NO.           KIND   DATE        APPLICATION NO.         DATE
     ---------------      ----   --------    --------------------    --------
     WO 2006015865         A1    20060216    WO 2005-EP8748          20050811
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ,
             LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA,
             NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK,
             SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU,
             ZA, ZM, ZW
```

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: GB 2004-18047 A 20040812

GI



I

AB Synergistic fungicidal compns. comprise the pyrazole derivs. I (R1 = CF3 or CHF2; H or Me) or I tautomers and one of a very large number of known fungicides.

IC ICM A01N043-56
ICS A01N061-00; A01N043-78; A01N043-653; A01N043-54; A01N043-36

CC 5-2 (Agrochemical Bioregulators)

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2006:147248 CAPLUS

DOCUMENT NUMBER: 144:186456

TITLE: Pyrazole derivative fungicides

INVENTOR(S): **Walter, Harald**; Zeun, Ronald; **Ehrenfreund, Josef**; **Tobler, Hans**; Corsi, Camilla; Lamberth, Clemens

PATENT ASSIGNEE(S): Syngenta Participations AG, Switz.

SOURCE: PCT Int. Appl., 32 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

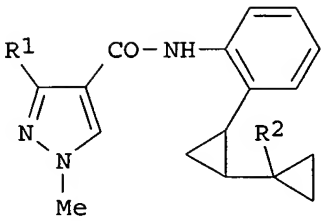
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006015866	A1	20060216	WO 2005-EP8752	20050811

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: GB 2004-18048 A 20040812

GI



I

AB The pyrazole derivs. I (R1 = trifluoromethyl or difluoromethyl; R2 = H or Me) or their tautomers are fungicides for plants and seeds.
CC 5-2 (Agrochemical Bioregulators)
REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2006:53749 CAPLUS
DOCUMENT NUMBER: 144:150025
TITLE: Process for the preparation of 4,4-difluoro-3-oxobutanoic acid esters
INVENTOR(S): **Walter, Harald**; Corsi, Camilla; **Ehrenfreund, Josef**; Lamberth, Clemens; **Tobler, Hans**
PATENT ASSIGNEE(S): Syngenta Participations A.-G., Switz.
SOURCE: PCT Int. Appl., 13 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006005612	A1	20060119	WO 2005-EP7635	20050713

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: GB 2004-15764 A 20040714
AB The present invention relates to a process for the preparation of title compds. F2CHCOCH2CO2R (R = C1-12 alkyl) by reaction of difluoroacetamides F2CHCONR1R2 (R1, R2 = independently C1-12 alkyl; or NR1R2 = alicyclic ring containing 4 to 7 carbon atoms, morpholino) with an acetic acid ester in the presence of a base. Thus, treatment of solution of N,N-diethyl-2,2-difluoroacetamide (prepared in 2 steps from dichloroacetyl chloride and dimethylamine) with ethanolic NaOEt in EtOAc gave 66% 4,4-difluoro-3-oxobutanoic acid Et ester after workup.

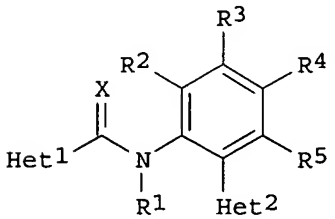
IC ICM C07C067-343
ICS C07C069-716
CC 23-17 (Aliphatic Compounds)
Section cross-reference(s): 45
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 4 OF 12 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:1354818 CAPLUS
DOCUMENT NUMBER: 144:88281
TITLE: Preparation of heterocyclic carboxamides with microbiocidal activity
INVENTOR(S): Lamberth, Clemens; Corsi, Camilla; **Ehrenfreund, Josef**; **Tobler, Hans**; **Walter, Harald**
PATENT ASSIGNEE(S): Syngenta Participations AG, Switz.
SOURCE: PCT Int. Appl., 152 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005123722	A1	20051229	WO 2005-EP6688	20050621

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: GB 2004-13970 A 20040622
OTHER SOURCE(S): MARPAT 144:88281
GI



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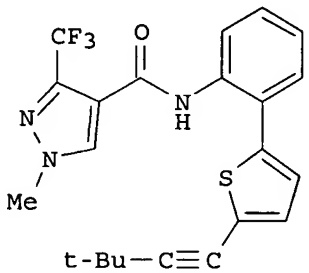

II

AB Title compds. I [Het1-2 = 5-6 membered heterocyclic ring; R1 = H, formyl, carboxyalkyl, etc.; R2-5 = H, halo, Me, CF3; X = O, S] are prepared For instance, II is prepared in 5 steps from 2-(tributylstannyl)thiophene, 1-iodo-2-nitrobenzene, 3,3-dimethyl-1-butyne and 1-methyl-3-

trifluoromethyl-1H-pyrazole-4-carboxylic acid. II when applied to plants inoculated with P. recondita nearly completely prevented infestation (0-5%). I are suitable for use as microbiocides.

IC ICM C07D403-12
ICS C07D409-12; C07D333-20; C07D231-14; C07D231-40; A01N043-56

CC 28-8 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 5

REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 5 OF 12 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:283496 CAPLUS
DOCUMENT NUMBER: 142:336464
TITLE: Preparation of heterocyclic substituted silicon compounds with microbiocidal activity
INVENTOR(S): **Ehrenfreund, Josef**; Lamberth, Clemens; **Tobler, Hans**; **Walter, Harald**
PATENT ASSIGNEE(S): Syngenta Participations Ag, Switz.
SOURCE: PCT Int. Appl., 68 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005028485	A1	20050331	WO 2004-EP10009	20040908
WO 2005028485	C1	20050609		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: GB 2003-22012 A 20030919
OTHER SOURCE(S): MARPAT 142:336464
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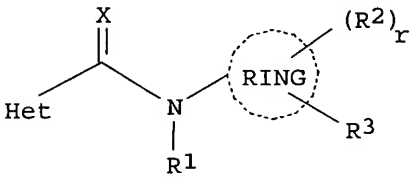


I

AB Preparation of fungicidal compds. I (X = O, S; RING = Ph, thienyl; Het = 5- or 6-membered heterocyclic ring containing one to three heteroatoms, each independently selected from O, N, S, the ring being substituted by one to

four groups R4; R1 = H, optionally substituted (C1-4)alkyl, formyl, optionally substituted (C1-4)alkylC(:O), optionally substituted (C1-4)alkylC(:O)O, optionally substituted (C1-4)alkoxy(C1-4)alkyl, optionally substituted allyl, optionally substituted propargyl or optionally substituted allenyl; R2 = independently, halo, optionally substituted (C1-4)alkyl, optionally substituted (C1-4)alkoxy or optionally substituted (C1-4)alkoxy(C1-4)alkyl; R3 = (CRaRb)m-Cy-(CRCRd)n-Y; R4 = independently, selected from halo, C1-3 alkyl, C1-3 haloalkyl, C1-3 alkoxy(C1-3)alkyl and cyano; Ra, Rb, Rc, Rd = independently, H, optionally substituted (C1-4)alkyl; Cy is an optionally substituted carbocyclic or heterocyclic 3-7 membered ring which may be saturated, unsatd. or aromatic and which optionally contains a silicon atom as a ring member; (CRaRb)m and (CRcRd)n may be bound either to the same carbon or silicon atom of Cy or to different atoms separated by 1, 2 or 3 ring members; Y = silyloxy etc.), useful as fungicides in agriculture (activity given), is described. Thus, reaction of N-methyl-3-difluoromethyl-4-chlorocarbonylpyrazole with 1,1-dimethyl-3-(2'-amino)phenylsilacyclohexane (preparation given) gave title compound which was used as fungicides (activity given).

IC ICM C07F007-08
ICS A01N055-00

CC 29-6 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 5, 10

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 6 OF 12 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:996168 CAPLUS
DOCUMENT NUMBER: 141:424106
TITLE: Preparation of 3-carbonylaminothiophenes as fungicides
INVENTOR(S): **Ehrenfreund, Josef**; **Walter, Harald**; **Tobler, Hans**; Lamberth, Clemens
PATENT ASSIGNEE(S): Syngenta Participations Ag, Switz.
SOURCE: PCT Int. Appl., 44 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

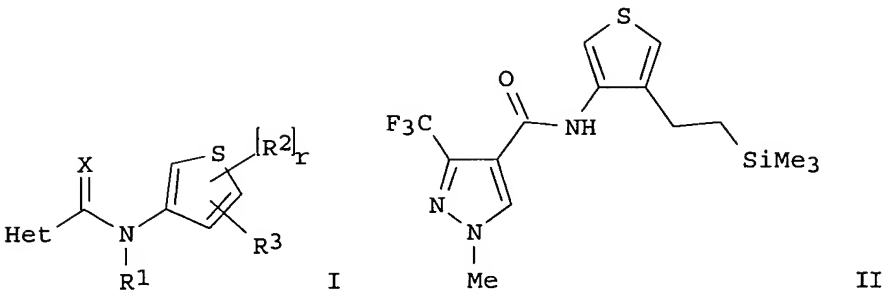
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004099195	A1	20041118	WO 2004-EP4194	20040421
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2524508	AA	20041118	CA 2004-2524508	20040421
EP 1620431	A1	20060201	EP 2004-728528	20040421
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				

PRIORITY APPLN. INFO.: GB 2003-10464 A 20030507
GB 2003-18920 A 20030812
GB 2004-4806 A 20040303

WO 2004-EP4194 W 20040421

OTHER SOURCE(S): MARPAT 141:424106

GI



I II

AB The title compds. I [Het = (un)substituted 5-6 membered heterocyclic ring containing 1-3 heteroatoms; R1 = H, alkyl, formyl, propargyl, etc.; R2 = halo, alkyl, alkoxy or alkoxyalkyl; R3 is either at position 2 or at position 4 of the thiophene ring and is an organic group containing 3-13 carbon atoms and at least one silicon atom and, optionally, 1-3 heteroatoms, and is optionally substituted by 1-4 halogen atoms; r = 0-2; X = O, S], useful in agriculture or horticulture for controlling or preventing infestation of plants by phytopathogenic microorganisms, preferably fungi, were prepared E.g., a multi-step synthesis of II, starting from 4-bromo-3-thiophenecarboxylic acid, was given. The compds. I were tested in various tests for fungicidal activity (data were given for representative compds. I).

IC ICM C07D409-12
ICS C07D417-12; C07D413-12; C07D411-12; C07D333-36; C07D333-28; A01N043-10

CC 27-8 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 5, 28

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 7 OF 12 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:565219 CAPLUS
DOCUMENT NUMBER: 141:123619
TITLE: Preparation of biphenyl derivatives and their use as fungicides
INVENTOR(S): **Ehrenfreund, Josef**; Lamberth, Clemens; **Tobler, Hans**; **Walter, Harald**
PATENT ASSIGNEE(S): Syngenta Participations Ag, Switz.
SOURCE: PCT Int. Appl., 102 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

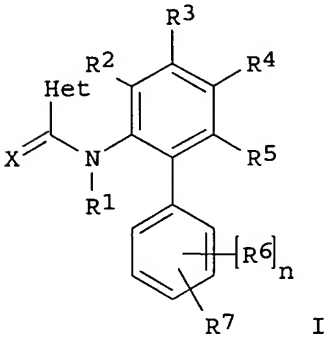
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004058723	A1	20040715	WO 2003-EP14248	20031215

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,

LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO,
NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ,
TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,
ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK,
TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

CA 2510528	AA	20040715	CA 2003-2510528	20031215
AU 2003300523	A1	20040722	AU 2003-300523	20031215
EP 1575922	A1	20050921	EP 2003-813891	20031215
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003016879	A	20051025	BR 2003-16879	20031215
NO 2005003558	A	20050725	NO 2005-3558	20050720
PRIORITY APPLN. INFO.:			GB 2002-30155 A	20021224
			WO 2003-EP14248 W	20031215

OTHER SOURCE(S): MARPAT 141:123619
GI



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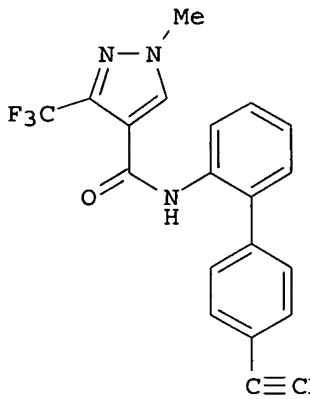

II

AB The title compds. [I; Het = (un)substituted 5-6 membered heterocyclic ring; R1 = H, CHO, CO(alkyl), CO2(alkyl), alkoxyalkylene, CO(alkylenoxy)alkyl, propargyl, allenyl; R2-R5 = H, halo, Me, CF3; R6 = halo, Me, CF3; R7 = (Z)mC.tplbond.CY1, (Z)mCY1:CY2Y3, trialkylsilyl; X = O, S; Y1-Y3 = H, halo, (un)substituted alkyl alkenyl, alkynyl, cycloalkyl, trialkylsilyl; Z = (un)substituted alkylene; m = 0-1; n = 0-2], useful in agriculture or horticulture for controlling or preventing infestation of plants by phytopathogenic microorganisms, preferably fungi, were prepared Thus, reacting 2-amino-4'-ethynylbiphenyl with 1-methyl-3-trifluoromethyl-4-chlorocarbonylpyrazole in the presence of pyridine in THF afforded 70% II which showed excellent fungicidal activity (biol. data given).

IC ICM C07D231-14
ICS C07D231-16; C07D207-34; C07D277-56; C07D263-34; C07D333-38; C07D307-68; C07D309-28; C07D327-06; C07D213-82; C07D239-28; C07D239-30; C07D237-24; C07C233-03; C07C211-45

CC 28-8 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 5

L27 ANSWER 8 OF 12 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:390242 CAPLUS
DOCUMENT NUMBER: 140:406731

TITLE: Preparation of N-(cyclopropylthienyl)carboxamides as fungicides

INVENTOR(S): **Ehrenfreund, Josef; Tobler, Hans; Walter, Harald**

PATENT ASSIGNEE(S): Syngenta Participations Ag, Switz.

SOURCE: PCT Int. Appl., 43 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004039799	A1	20040513	WO 2003-EP11805	20031024
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2501739	AA	20040513	CA 2003-2501739	20031024
AU 2003286140	A1	20040525	AU 2003-286140	20031024
EP 1556377	A1	20050727	EP 2003-776869	20031024
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003015857	A	20050920	BR 2003-15857	20031024
JP 2006508089	T2	20060309	JP 2004-547558	20031024
US 2006030567	A1	20060209	US 2005-532847	20050427
PRIORITY APPLN. INFO.:			GB 2002-25554 A	20021101
			WO 2003-EP11805 W	20031024

OTHER SOURCE(S): MARPAT 140:406731

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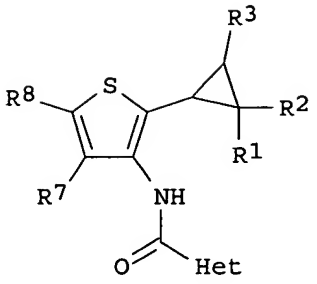

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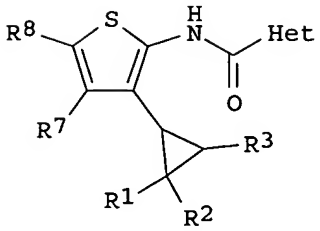

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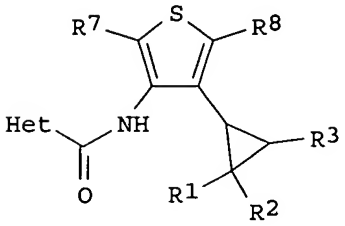
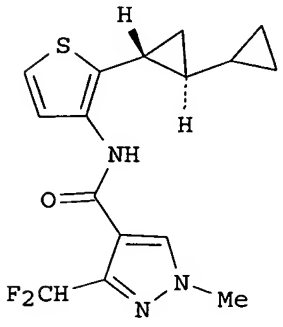


III



IV

AB A fungicidally active compound I, II, or III [wherein Het = (un)substituted 5- or 6-membered heterocyclic ring containing one to three O, N, and/or S atoms, provided that the ring is not 1,2,3-triazole; R1 and R2 = independently H, halo, or Me; R3 = (un)substituted (cyclo)alkyl, alkenyl, alkynyl, Ph, heterocyclyl; R7 and R8 = independently H, halo, or (halo)alkyl] were prepared for use as active ingredients in agricultural or horticultural compns. for controlling or preventing infestation of plants by phytopathogenic microorganisms, preferably fungi. For example, 3-difluoromethyl-1-methyl-1H-pyrazole-4-carboxylic acid was amidated with [2-(bicyclopropyl-2-yl)thiophen-3-yl]amine in the presence of TEA and N,N-bis(2-oxooxazolidinyl)phosphinic acid chloride in CH2Cl2 to give trans-IV (97% purity). The latter showed excellent activity against Puccinia recondita on wheat (0-5% infestation) and showed good activity against Podosphaera leucotricha on apple, Venturia inaequalis on apple, Erysiphe graminis on barley, Pyrenophora teres on barley, Alternaria solani on tomato, and Uncinula necator on grape (<20% infestation for each).

IC ICM C07D409-12
ICS C07D411-12; C07D417-12; C07D333-36; A01N043-56; A01N043-36; A01N043-78; A01N043-40; A01N043-32

CC 27-8 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 10

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 9 OF 12 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:354949 CAPLUS
DOCUMENT NUMBER: 140:375164
TITLE: Preparation of heterocyclocarboxamides and tricyclic amines as fungicides
INVENTOR(S): **Ehrenfreund, Josef; Tobler, Hans; Walter, Harald**

PATENT ASSIGNEE(S): Syngenta Participations A.-G., Switz.
SOURCE: PCT Int. Appl., 58 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004035589	A1	20040429	WO 2003-EP11388	20031014
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2498851	AA	20040429	CA 2003-2498851	20031014
AU 2003280376	A1	20040504	AU 2003-280376	20031014
EP 1556385	A1	20050727	EP 2003-772217	20031014
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003014875	A	20050802	BR 2003-14875	20031014
NO 2005002201	A	20050527	NO 2005-2201	20050504
PRIORITY APPLN. INFO.:			GB 2002-24316 A	20021018
			WO 2003-EP11388 W	20031014

OTHER SOURCE(S): MARPAT 140:375164
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The invention relates to fungicidally active heterocyclocarboxamides (shown as I; e.g. II; Het is a 5- or 6-membered heterocyclic ring containing 1-3 heteroatoms = O, N and S, provided that the ring is not 1,2,3-triazole, the ring being substituted by groups R8, R9 and R10; X is a single or double bond; Y is O, S, N(R11) or (CR12R13)(CR14R15)m(CR16R17)n; m is 0 or 1; n is 0 or 1; and R1 to R17 each, independently, have a range of values) and tricyclic amines (shown as III; e.g. IV; variables defined below) to the preparation of these compds., to novel intermediates used in the preparation of these compds., to agrochem. compns. which comprise at least one of the novel compds. as active ingredient, to the preparation of the compns. mentioned and to the use of the active ingredients or compns. in agriculture or horticulture for controlling or preventing infestation of plants by phytopathogenic microorganisms, preferably fungi. Although the methods of preparation are not claimed, example prepns. and/or characterization data are included for .apprx.150 examples of I. For example, IV was prepared (94 %) by hydrogenation of 1,4-dimethyl-5-nitro-1,4-dihydro-1,4-epoxynaphthalene; reaction of IV with 1-methyl-4-trifluoromethyl-1H-pyrrole-3-carboxylic acid/oxalyl chloride in DMF gave II (59 %); II was N-alkylated with 3-bromo-1-propyne (50 %). Examples of I are listed that are effective against the following: brownrust on wheat, powdery mildew on apple, scab on apple, powdery mildew on barley, botrytis on grapes, botrytis on

tomatoes, net blotch on barley, early blight on tomatoes, powdery mildew on grapes, fusarium head blight on wheat, take-all on wheat, brownrust on wheat, sheath blight on rice, and septoria leaf spot on wheat. For III: Y is O or S; and R4, R5, R6 and R7 are each C(O)OCH3; or Y is N(R11) or (CR12R13)(CR14R15)m(CR16R17)n; R11 is benzyl (in which the Ph group is (un)substituted with up to three halo, C1-4 alkyl, C1-4 haloalkyl and C1-4-alkoxy); and R12 and R13 together with the C atom to which they are attached form a 3-5 membered carbocyclic ring ((un)substituted by ≤3 Me groups and containing 1 or 2 heteroatoms = O and N); other variables are as defined earlier.

IC ICM C07D487-08
ICS C07D493-08; C07D495-08; C07D207-34; C07D231-14; C07D213-78; C07D277-56; C07D263-34; C07D327-06; A01N043-36; A01N043-32; A01N043-50

CC 28-8 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 5, 27

REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

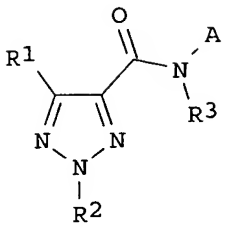
L27 ANSWER 10 OF 12 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:182852 CAPLUS
DOCUMENT NUMBER: 140:235719
TITLE: Preparation of triazolylcarboxylic acid derivatives with antifungal activity for agricultural use
INVENTOR(S): **Ehrenfreund, Josef; Tobler, Hans; Walter, Harald**
PATENT ASSIGNEE(S): Syngenta Participations A.-G., Switz.
SOURCE: PCT Int. Appl., 82 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004018438	A2	20040304	WO 2003-EP9111	20030818
WO 2004018438	A3	20040826		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2494263	AA	20040304	CA 2003-2494263	20030818
AU 2003253417	A1	20040311	AU 2003-253417	20030818
EP 1539717	A2	20050615	EP 2003-792351	20030818
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003013686	A	20050621	BR 2003-13686	20030818
CN 1678593	A	20051005	CN 2003-819890	20030818
JP 2006502244	T2	20060119	JP 2005-501204	20030818

PRIORITY APPLN. INFO.:
GB 2002-19612 A 20020822
GB 2003-10464 A 20030507
WO 2003-EP9111 W 20030818

OTHER SOURCE(S): MARPAT 140:235719

GI



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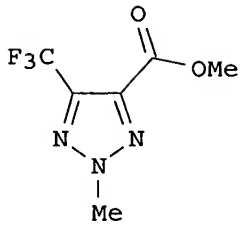


II

AB Title compds. I [A = ortho-substituted aryl or heteroaryl ring system; R1 = halo, CN, NO2, alkyl, haloalkyl, alkoxy, haloalkoxy, (un)substituted alkene, etc.; R2 = alkyl, haloalkyl, alkoxyalkyl, etc.; R3 = H, (un)substituted-alkyl, -propargyl, -alkoxy, etc.] were prepared and disclosed as having antifungal activity. Thus, e.g., II was prepared via methylation of 1,2,3-triazole-4,5-dicarboxylic acid di-Me ester, with subsequent monohydrolysis and fluorination of the carboxylic acid moiety to the trifluoromethyl moiety. I were tested against 9 different agriculturally relevant fungi with varying degrees of efficacy observed Addnl., a composition of I with a suitable carrier for controlling microorganisms and preventing attack and infestation of plants therewith is claimed.

IC ICM C07D249-04
ICS C07D409-12; C07D405-12; C07D403-12; C07D307-00; C07D209-94; A01N043-647

CC 28-10 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 5, 10

L27 ANSWER 11 OF 12 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:777810 CAPLUS
DOCUMENT NUMBER: 139:277000
TITLE: Siliconated phenyl amides derivatives useful as microbiocide
INVENTOR(S): **Ehrenfreund, Josef**; Jung, Pierre Joseph Marcel; **Tobler, Hans**; **Walter, Harald**
PATENT ASSIGNEE(S): Syngenta Participations A.-G., Switz.
SOURCE: PCT Int. Appl., 42 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

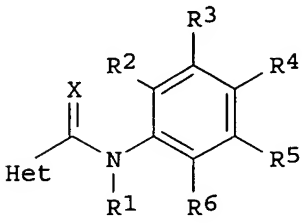
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003080628	A1	20031002	WO 2003-IB1110	20030321

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,

	FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,						
	BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG						
CA 2477396		AA	20031002	CA 2003-2477396			20030321
AU 2003212576		A1	20031008	AU 2003-212576			20030321
BR 2003008759		A	20041228	BR 2003-8759			20030321
EP 1490378		A1	20041229	EP 2003-708401			20030321
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,						
	IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK						
JP 2005520863		T2	20050714	JP 2003-578382			20030321
CN 1642963		A	20050720	CN 2003-806592			20030321
US 2005182107		A1	20050818	US 2003-509607			20030321
EG 23440		A	20050903	EG 2003-286			20030326
PRIORITY APPLN. INFO.:				GB 2002-7253		A	20020327
				WO 2003-IB1110		W	20030321

OTHER SOURCE(S): CASREACT 139:277000; MARPAT 139:277000

GI



I

AB The preparation of title compds., I (Het = 5- or 6-membered heterocyclic ring containing one to three heteroatoms, each independently selected from O, N, and S, the ring being substituted by groups R7, R8, R9; R1 = H, (C1-4)alkylC(:O), (C1-4)alkylC(:O)O, (C1-4)alkoxy(C1-4)alkyl, substituted allyl, substituted propargyl or substituted allenyl; R2, R3, R4, R5 = H, halo, (C1-4)alkoxy(C1-4)alkoxy, (C1-4)alkoxy(C1-4)alkyl; R6 = C1-13 group containing at least one silicon atom and, 1-3 heteroatoms, each independently selected from O, N, S, and is substituted by 1-4 independently selected halogen atoms; R7, R8, R9 = H, halo, C1-3 alkyl, C1-3 haloalkyl, C1-3alkoxy(C1-3)alkyl, cyano, where at least one of R7, R8, R9 is not hydrogen; X = O, S; or an N-oxide thereof; and when present, each optional substituent on alkyl moieties, allyl, propargyl and allenyl is, independently, selected. from halo, OH, cyano, MeO2CO, EtO2CO, MeO, EtO, methylsulfonyl, ethylsulfonyl, diflouromethoxy, trifluoromethoxy, trifluorothiomethoxy), useful as fungicides, is described. The activity of prepared compds. were tested against Puccinia recondita (wheat), Podosphaera leucotricha (apple), Venturia inaequalis (apple), Erysiphe graminis (barley), Botrytis cinerea (tomato), and Septoria nodorum (wheat).

IC ICM C07F007-08
ICS A01N055-00; A01N055-10

CC 29-6 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 5, 10, 25

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 12 OF 12 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:719453 CAPLUS
DOCUMENT NUMBER: 139:246007

TITLE: Preparation of heterocyclic ortho-cyclopropyl-carboxanilides and their use as fungicides

INVENTOR(S): **Ehrenfreund, Josef; Tobler, Hans; Walter, Harald**

PATENT ASSIGNEE(S): Syngenta Participations Ag, Switz.

SOURCE: PCT Int. Appl., 40 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003074491	A1	20030912	WO 2003-IB687	20030221
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
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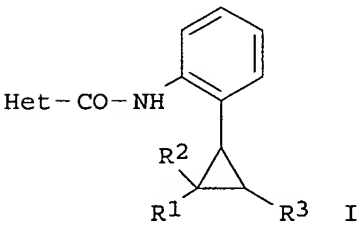
CA 2477931	AA	20030912	CA 2003-2477931	20030221
AU 2003208490	A1	20030916	AU 2003-208490	20030221
EP 1480955	A1	20041201	EP 2003-706779	20030221
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003008230	A	20041228	BR 2003-8230	20030221
CN 1639128	A	20050713	CN 2003-805172	20030221
JP 2005532271	T2	20051027	JP 2003-572960	20030221
EG 23424	A	20050712	EG 2003-204	20030301
US 2005221989	A1	20051006	US 2005-506918	20050428

PRIORITY APPLN. INFO.:
GB 2002-5127 A 20020305
GB 2003-705 A 20030113
WO 2003-IB687 W 20030221

OTHER SOURCE(S): MARPAT 139:246007

GI



I

AB Heterocyclic o-cyclopropyl-carboxanilides (shown as I; e.g. N-[2-(2-isopropylcyclopropyl)phenyl]-1-methyl-3-trifluoromethyl-1H-pyrazole-4-carboxamide; Het is a 5- or 6-membered heterocyclic ring containing 1-3 heteroatoms, = O, N and S, the ring being substituted by groups R4, R5 and R6; R1 is H or halo; R2 is H or halo; R3 is (un)substituted C2-12 alkyl, (un)substituted C2-12 alkenyl, (un)substituted C2-12 alkynyl, (un)substituted C3-12 cycloalkyl, (un)substituted Ph or (un)substituted

heterocyclyl; and R4, R5 and R6 = H, halo, cyano, nitro, C1-4 haloalkyl, C1-4 alkoxyl (C1-4) alkyl and C1-4 haloalkoxy (C1-4) alkyl, provided that at least one of R4, R5 and R6 is not H) are claimed. I have plant-protective properties and are suitable for protecting plants against infestations by phytopathogenic microorganisms. Three example prepns. are included. To prepare N-[2-(2-isobutylcyclopropyl)phenyl]-1-methyl-4-trifluoromethyl-1H-pyrrole-3-carboxamide, (2-isobutylcyclopropyl)benzene (17.4 g) in Ac2O was nitrated to give a mixture of regioisomers that was hydrogenated over 5 % Pt/C to give a cis/trans mixture of 2-(2-isobutylcyclopropyl)phenylamine (6.38 g) after workup; the anilines (0.35 g) were condensed with 1-methyl-4-trifluoromethylpyrrole-3-carboxylic acid after the latter was reacted with oxalyl chloride in CH2Cl2 for 3 h at room temperature to give 0.52 g of the final product. More than 300 examples of I are tabulated, most without characterization data, and general statements are made as to the activity of some or all of them against Puccinia recondita/wheat (Brownrust on wheat), Podosphaera leucotricha/apple (Powdery mildew on apple), Venturia inaequalis/apple (Scab on apple), Erysiphe graminis/barley (Powdery mildew on barley), Botrytis cinerea/apple (Botrytis on apple fruits), Botrytis cinerea/grape (Botrytis on grapes), Botrytis cinerea/tomato (Botrytis on tomatoes), Pyrenophora teres/barley (Net blotch on barley), and Septoria nodorum/wheat (Septoria leaf spot on wheat). For example, infestation of wheat by brownrust is prevented virtually completely (0-5 % infestation) by N-[2-(2-isopropylcyclopropyl)phenyl]-1-methyl-3-trifluoromethyl-1H-pyrazole-4-carboxamide.

IC ICM C07D231-14
ICS C07D231-16; C07D409-12; C07D405-12; C07D207-34; C07D277-56; C07D417-12; C07D213-82; C07D327-06; C07D411-12; A01N043-56; A01N043-36; A01N043-78; A01N043-40; A01N043-32

CC 28-1 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 5

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> □

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FILE LAST UPDATED: 20 Mar 2006 (20060320/ED)

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http://www.cas.org/infopolicy.html
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=> d que nos L11
L1              STR
L3       546562 SEA FILE=REGISTRY ABB=ON  PLU=ON  SC4/ES
L5         2304 SEA FILE=REGISTRY SUB=L3 SSS FUL L1
L8              STR
L10         630 SEA FILE=REGISTRY SUB=L5 SSS FUL L8
L11           1 SEA FILE=CAPLUS ABB=ON  PLU=ON  L10

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L12          ANALYZE L10 1- LC :       4 TERMS

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FILE LAST UPDATED 18 MARCH 2006 (20060318/UP)

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HELP SPA, HELP SPBC, HELP SPDH, HELP SPIN, HELP SPOP, and HELP SPQZ.
For the list of current catalogs, enter HELP CTA, HELP CTBC, HELP
CTDH, HELP CTIN, HELP CTOP, and HELP CTQZ.

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liable for any loss of profit, goodwill or any other damages arising
out of the use of this database.

CHEMCATS now contains more than 8 million records.  See HELP CONTENT
and NEWS FILE for details.

=> d que nos L23
L1              STR
L3       546562 SEA FILE=REGISTRY ABB=ON  PLU=ON  SC4/ES
L5         2304 SEA FILE=REGISTRY SUB=L3 SSS FUL L1
L8              STR
L10         630 SEA FILE=REGISTRY SUB=L5 SSS FUL L8
L23           2 SEA FILE=CHEMCATS ABB=ON  PLU=ON  L10


=> d iall L23 1-2
'IALL' IS NOT A VALID FORMAT FOR FILE 'CHEMCATS'
```

There is only reference in CAPlus; it contains 630 structures.

(Chemical Catalogs)

The following are valid formats:

The default display format is IDE.

```
ALL ---- AN, CO, PD, ON, CN, RN, ST, Purity, Impurity, product
         identifiers, product notes, STR, product text
         (properties, regulatory information, references, prices,
         warnings, miscellaneous fields), CO, CA, CY, TX
         (products, terms, and conditions; products and services;
         packaging and shipping; safety and handling; other
         supplier information)
COMP --- AN, CO, PD, CO, TX
IDE ---- AN, CO, PD, ON, CN, RN, LSF, ST, STR
MISC --- AN, miscellaneous product information fields
PINFO -- AN, pricing information text
PRICE -- AN, prices, quantities
PROD --- AN, product text
PROP --- AN, properties
REF ---- AN, references
REGS --- AN, regulatory information
SAFE --- AN, product warnings
SINFO -- AN, safety text
HIT ---- All fields containing hit terms
KWIC --- All hit terms plus 20 words on either side
OCC ---- List of display fields containing hit terms
```

Hit terms will be highlighted in all displayable fields.

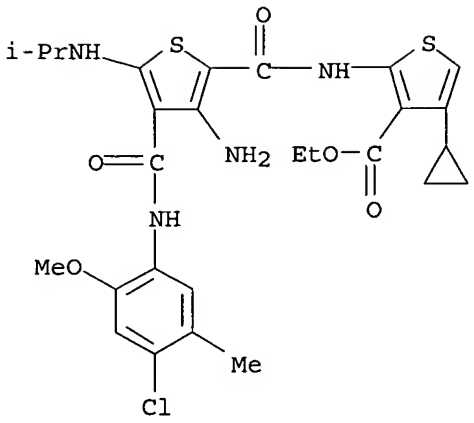
To display a particular field or fields, enter the display field codes. For a list of display field codes, enter 'HELP DFIELDS' at an arrow prompt (=>). Examples include: 'KWIC'; 'CN RN'; 'IDE CO'. You may specify the formats and fields in any order, and the information will be displayed in the same order as the format specification.

The same formats (except for HIT, KWIC, and OCC) may be used with the DISPLAY ACC command to display the record for a specified Accession Number.

pleare disregard

ENTER DISPLAY FORMAT (IDE):all

L23 ANSWER 1 OF 2 CHEMCATS COPYRIGHT 2006 ACS on STN
Accession No. (AN): 2005:3316726 CHEMCATS
Catalog Name (CO): Ambinter Stock Screening Collection
Publication Date (PD): 3 Jul 2005
Order Number (ON): T0517-2119
Chemical Name (CN): 3-Thiophenecarboxylic acid, 2-[[[3-amino-4-[[(4-chloro-2-methoxy-5-methylphenyl)amino]carbonyl]-5-[(1-methylethyl)amino]-2-thienyl]carbonyl]amino]-4-cyclopropyl-, ethyl ester
CAS Registry No. (RN): **734536-21-1**
Supplementary Term (ST): CHEMICAL LIBRARY
Structure :



PRICES

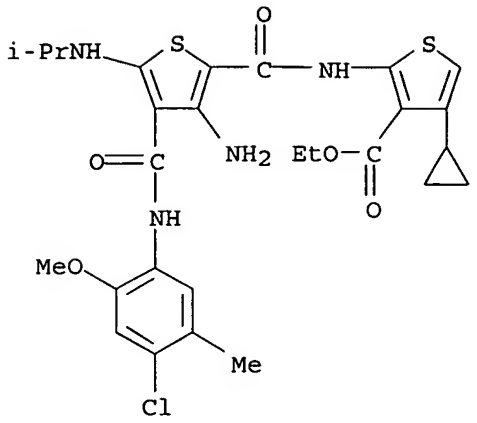
Quantity : milligram quantities, Price: contact supplier

COMPANY INFORMATION

Ambinter
50, avenue de Versailles
Paris, F-75016
France

Phone: (33-1) 45 24 48 60
Fax: (33-1) 45 24 62 41
Email: ambinter@compuserve.com
Web: http://www.ambinter.com

L23 ANSWER 2 OF 2 CHEMCATS COPYRIGHT 2006 ACS on STN
Accession No. (AN): 2005:133047 CHEMCATS
Catalog Name (CO): Enamine Screening Library
Publication Date (PD): 24 Jan 2006
Order Number (ON): T0517-2119
Chemical Name (CN): 3-Thiophenecarboxylic acid, 2-[[[3-amino-4-[[(4-chloro-2-methoxy-5-methylphenyl)amino]carbonyl]-5-[(1-methylethyl)amino]-2-thienyl]carbonyl]amino]-4-cyclopropyl-, ethyl ester
CAS Registry No. (RN): **734536-21-1**
Supplementary Term (ST): CHEMICAL LIBRARY
Structure :



PRICES

Quantity : milligram quantities, Price: contact supplier

COMPANY INFORMATION

Enamine
23 Alexandra Matrosova Street
Kiev, 01103
Ukraine

Phone: +380 44 537 32 18
Fax: +380 44 537 32 53
Email: enamine@enamine.net
Web: http://www.enamine.net

=> file marpat
FILE 'MARPAT' ENTERED AT 15:18:39 ON 21 MAR 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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FILE CONTENT: 1961-PRESENT VOL 144 ISS 12 (20060317/ED)

SOME MARPAT RECORDS ARE DERIVED FROM INPI DATA FOR 1961-1987

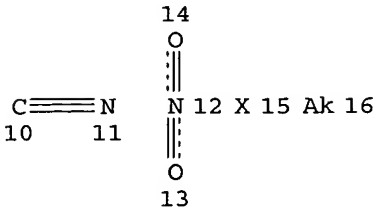
MOST RECENT CITATIONS FOR PATENTS FROM MAJOR ISSUING AGENCIES
(COVERAGE TO THESE DATES IS NOT COMPLETE):

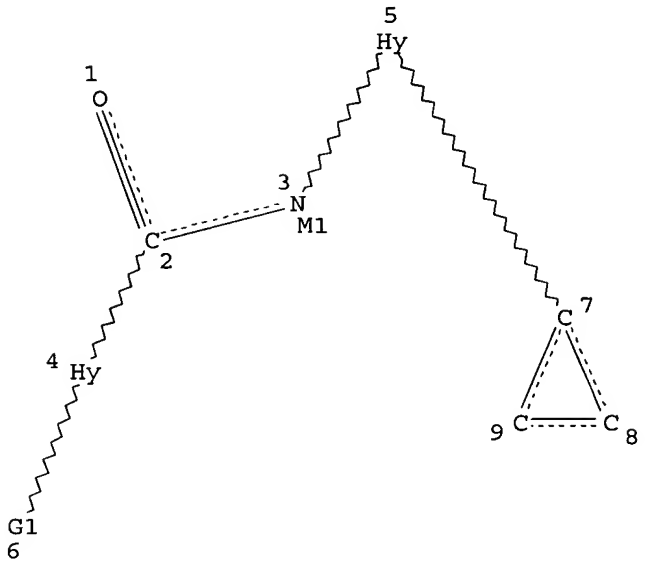
US 2006035965 16 FEB 2006
DE 102004030305 12 JAN 2006
EP 1614691 11 JAN 2006
JP 2006008639 12 JAN 2006
WO 2006012333 02 FEB 2006
GB 2415429 28 DEC 2005
FR 2873371 27 JAN 2006
RU 2267521 10 JAN 2006
CA 2472818 30 DEC 2005

Expanded G-group definition display now available.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

=> d stat que L22
L8 STR





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NSPEC IS C AT 1
NSPEC IS C AT 2
NSPEC IS C AT 3
NSPEC IS C AT 4
NSPEC IS C AT 5
NSPEC IS C AT 6
NSPEC IS R AT 7
NSPEC IS R AT 8
NSPEC IS R AT 9
DEFAULT MLEVEL IS ATOM
MLEVEL IS CLASS AT 10 11 12 13 14 15 16
GGCAT IS MCY LOC AT 4
GGCAT IS MCY LOC LOQ UNS AT 5
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS E4 C E0 N E0 O E1 S AT 5

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 16

STEREO ATTRIBUTES: NONE
L21 6 SEA FILE=MARPAT SSS FUL L8
L22 5 SEA FILE=MARPAT ABB=ON PLU=ON L21/COM

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FILE 'CAPLUS' ENTERED AT 15:19:24 ON 21 MAR 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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COPYRIGHT (C) 2006 AMERICAN CHEMICAL SOCIETY (ACS)

FILE 'MARPAT' ENTERED AT 15:19:24 ON 21 MAR 2006
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COPYRIGHT (C) 2006 American Chemical Society (ACS)
PROCESSING COMPLETED FOR L11
PROCESSING COMPLETED FOR L22
L29             5 DUP REM L11 L22 (1 DUPLICATE REMOVED)
                  ANSWER '1' FROM FILE CAPLUS
                  ANSWERS '2-5' FROM FILE MARPAT

=> d ibib abs L29 1; d ibib abs hit L29 2-5

L29  ANSWER 1 OF 5  CAPLUS  COPYRIGHT 2006 ACS on STN  DUPLICATE 1
ACCESSION NUMBER:         2004:390242  CAPLUS
DOCUMENT NUMBER:          140:406731
TITLE:                    Preparation of N-(cyclopropylthienyl)carboxamides as
                          fungicides
INVENTOR(S):              Ehrenfreund, Josef; Tobler, Hans; Walter, Harald
PATENT ASSIGNEE(S):       Syngenta Participations Ag, Switz.
SOURCE:                   PCT Int. Appl., 43 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.           KIND   DATE        APPLICATION NO.         DATE
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     WO 2004039799         A1    20040513    WO 2003-EP11805         20031024
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             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE,
             GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK,
             LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ,
             OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM,
             TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
             FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
             BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     CA 2501739            AA    20040513    CA 2003-2501739         20031024
     AU 2003286140         A1    20040525    AU 2003-286140          20031024
     EP 1556377            A1    20050727    EP 2003-776869          20031024
         R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
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     BR 2003015857         A     20050920    BR 2003-15857           20031024
     JP 2006508089         T2    20060309    JP 2004-547558          20031024
     US 2006030567         A1    20060209    US 2005-532847          20050427
PRIORITY APPLN. INFO.:                       GB 2002-25554        A  20021101
                                             WO 2003-EP11805      W  20031024

OTHER SOURCE(S):          MARPAT 140:406731
GI
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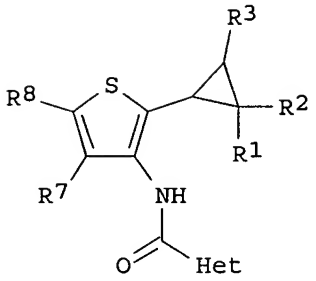
This reference contains 630 structures hit-on. They have not been printed here.

(application inventors)



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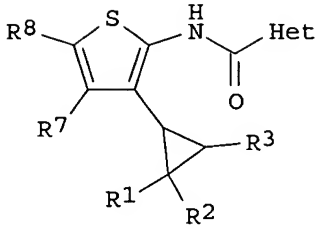

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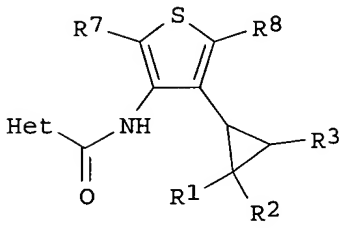

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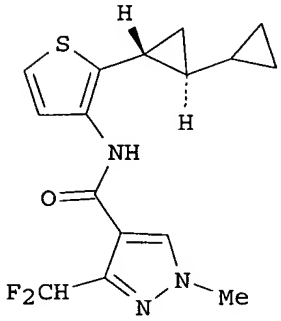

IV

AB A fungicidally active compound I, II, or III [wherein Het = (un)substituted 5- or 6-membered heterocyclic ring containing one to three O, N, and/or S atoms, provided that the ring is not 1,2,3-triazole; R1 and R2 = independently H, halo, or Me; R3 = (un)substituted (cyclo)alkyl, alkenyl, alkynyl, Ph, heterocyclyl; R7 and R8 = independently H, halo, or (halo)alkyl] were prepared for use as active ingredients in agricultural or horticultural compns. for controlling or preventing infestation of plants by phytopathogenic microorganisms, preferably fungi. For example, 3-difluoromethyl-1-methyl-1H-pyrazole-4-carboxylic acid was amidated with [2-(bicyclopropyl-2-yl)thiophen-3-yl]amine in the presence of TEA and N,N-bis(2-oxooxazolidinyl)phosphinic acid chloride in CH2Cl2 to give trans-IV (97% purity). The latter showed excellent activity against Puccinia recondita on wheat (0-5% infestation) and showed good activity against Podosphaera leucotricha on apple, Venturia inaequalis on apple, Erysiphe graminis on barley, Pyrenophora teres on barley, Alternaria solani on tomato, and Uncinula necator on grape (<20% infestation for each).

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L29 ANSWER 2 OF 5 MARPAT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 142:392408 MARPAT
TITLE: Preparation of cyclic diamines and derivatives as factor Xa inhibitors
INVENTOR(S): Qiao, Jennifer X.
PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
SOURCE: PCT Int. Appl., 117 pp.

CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005032490	A2	20050414	WO 2004-US32990	20041007
WO 2005032490	A3	20050728		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

US 2005085511	A1	20050421	US 2004-959724	20041007
PRIORITY APPLN. INFO.:			US 2003-509587P	20031008

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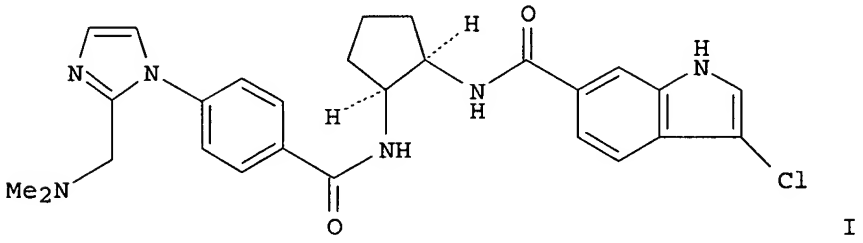


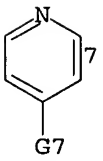
I

AB Title compds., e.g., I are prepared For instance I is prepared in 9 steps from (1S,2S)-1-amino-2-benzyloxycyclopentane, 3-chloro-1H-indole-6-carboxylic acid, 4-iodobenzoic acid Me ester and (1H-imidazol-2-ylmethyl)dimethylamine. Compds. of the invention exhibit Ki of ≤ 10 μM for factor Xa and are useful for the treatment of thromboembolic disorders.

MSTR 1

G1—G2—G3—G4—G5—G20
1 2 3 4 5 831

G1 = Ph (opt. substd. by G6) / 7 / 16 / 22 / 30 / 35 / 59 / 80 / 113 / 124 / 134 / 146 / 157 / 169 / 180 / 190 / 195 / 206 / 216 / 231 / 242 / 253 / 267 / 278 / 289 / 299 / 310 / 321 / 332 / 342 / 352 / 362 / 372 / 382 / 392 / 402 / 412 / 422 / 432 / 442 / 452 / 462 / 472 / 482 / 489 / 500 / 511 / 522 / 533 / 544 / 549 / 567 / 578 / 581 / 588 / 596 / 606 / 617 / 635 / 645 / 657 / 668 / 678 / 684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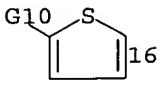
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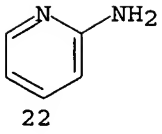
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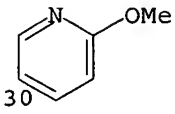
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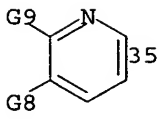
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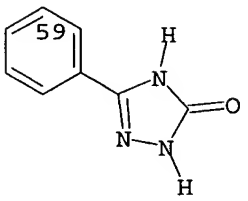
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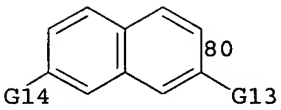
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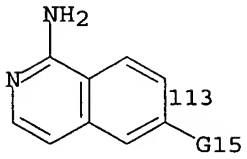
G13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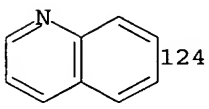
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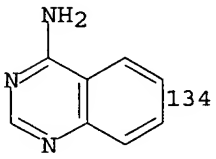
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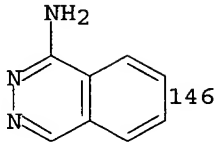
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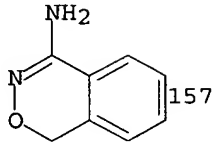
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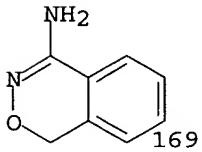
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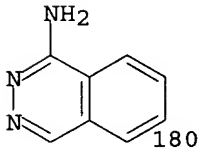
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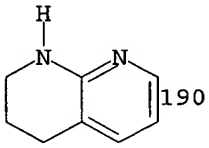
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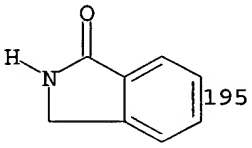
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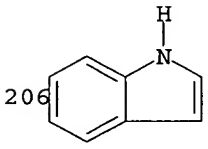
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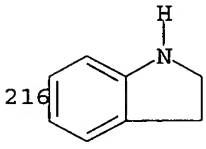
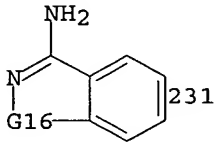
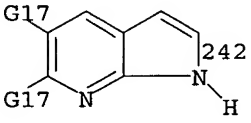
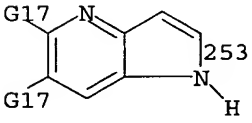
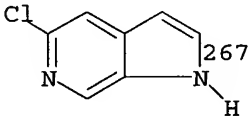
N
206

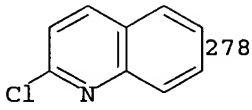

H
N
216


NH2
N
G16
231


G17
242
G17
N
N
H


G17
N
253
N
G17
H


Cl
267
N
N
H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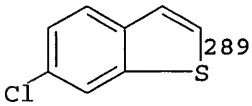
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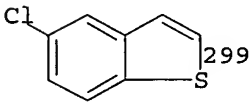
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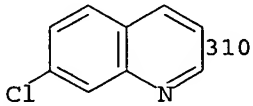
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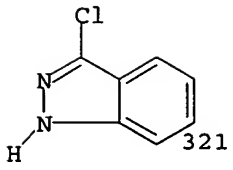

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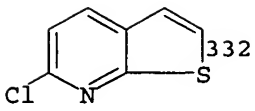

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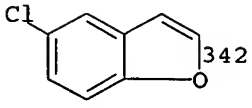

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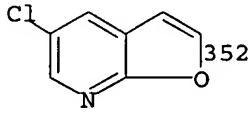

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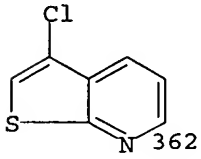

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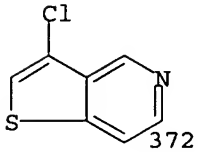

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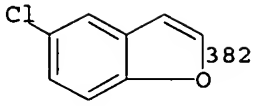

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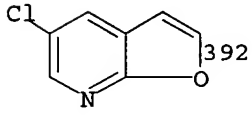

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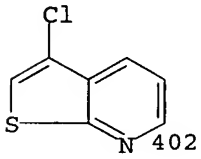

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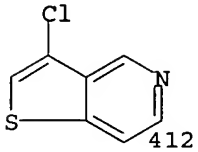

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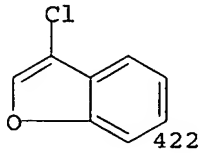

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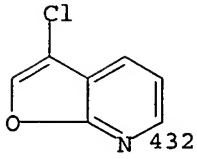

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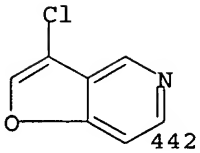

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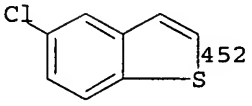

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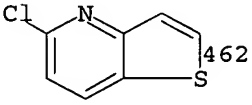

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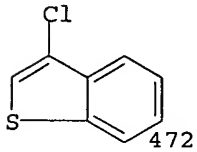

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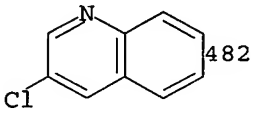

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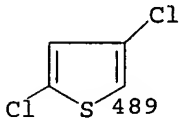

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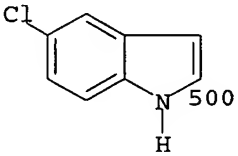

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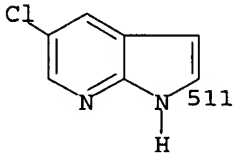

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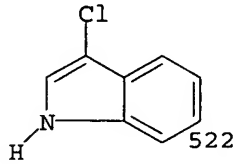

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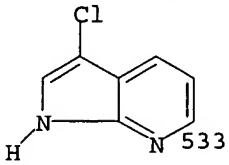

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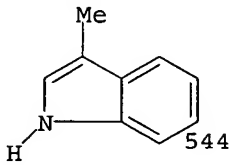

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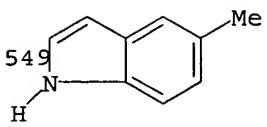
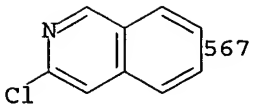
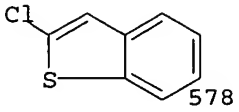
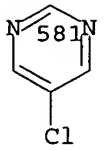
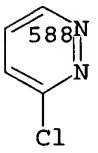
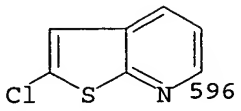


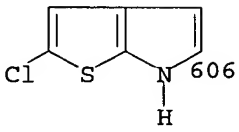


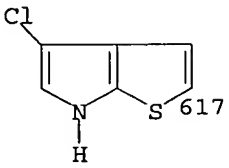


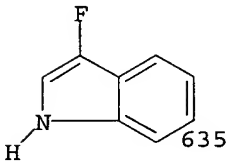


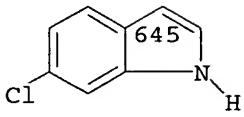


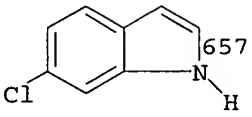


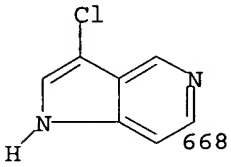


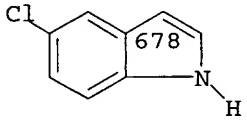


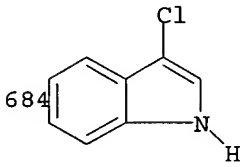












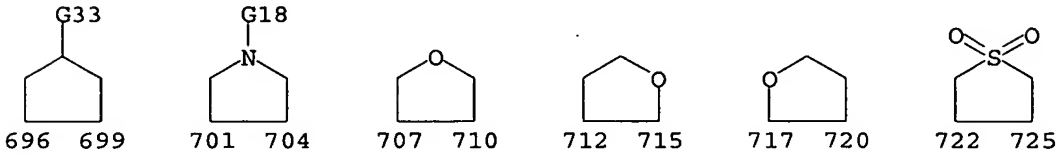
G2 = **43-1 42-3** / 44-1 45-3 / 46-1 47-3 / 48-1 50-3 / 51-1 54-3 / 55-1 56-3 / 57-1 58-3

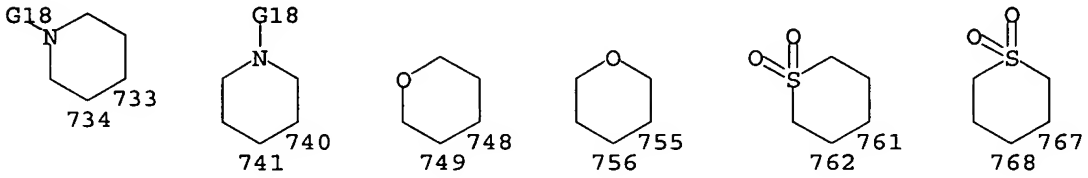
$\overset{43}{C}(O)\overset{42}{CH_2}$ $\overset{44}{HN}\overset{45}{-\!-}G11$ $G11\overset{46}{-}\overset{47}{NH}$ $\overset{48}{HN}\overset{50}{-\!-}C(O)-NH$ $\overset{51}{HN}\overset{54}{-\!-}C(O)-C(O)-NH$

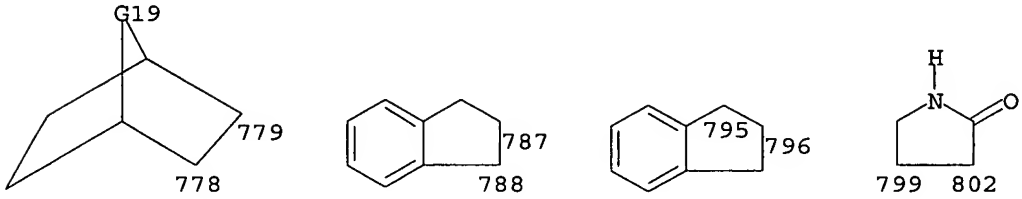
$O_2\overset{55}{S}\overset{56}{-\!-}NH$ $G12\overset{57}{-}\overset{58}{CH_2}$

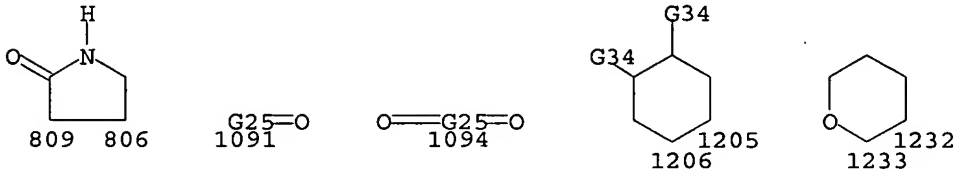
G3 = any ring <containing 5-6 atoms, 0-1 heteroatom, zero or more N, zero or more O, zero or more S (no other heteroatoms), attached through 2 C, bonds all single, 5- to 6-membered monocyclic ring> / 1091 / 1094 / any ring <containing 9-10 atoms, 0-2 heteroatoms, 0-2 N, 0-1 O, 0-1 S (no other heteroatoms), attached through 2 C, bicyclic, 5- or 6-membered rings only> / (Specifically claimed: 696-2 699-4 / **701-2 704-4** / 707-2 710-4 / 712-2 715-4 / 717-2 720-4 / 722-2 725-4 / 734-2 733-4 / 741-2 740-4 / 749-2 748-4 / 756-2 755-4 / 762-2 761-4 / 768-2 767-4 / 778-2 779-4 / 788-2 787-4 / 795-2 796-4 / 799-2 802-4 / 809-2 806-4) /

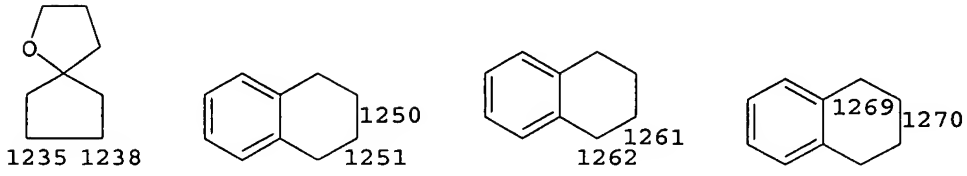
(Examples: 1206-2 1205-4 / 1233-2 1232-4 / 1235-2 1238-4 /
1262-2 1261-4 / 1251-2 1250-4 / 1270-2 1269-4 /
1274-2 1273-4 / 1282-2 1281-4 / 1290-2 1289-4 /
1298-2 1301-4 / 1308-2 1307-4)

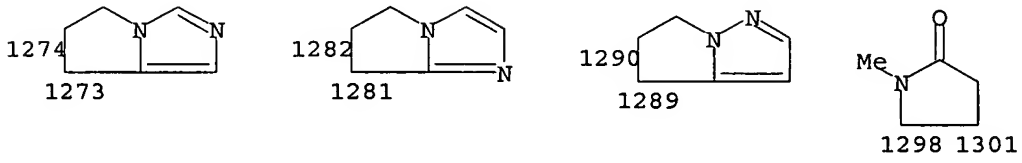


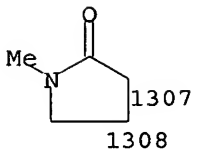




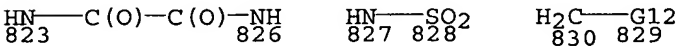




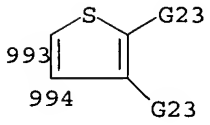


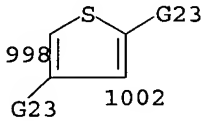


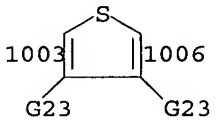
G4 = 814-3 815-5 / 816-3 817-5 / **818-3 819-5** /
820-3 822-5 / 823-3 826-5 / 827-3 828-5 / 830-3 829-5

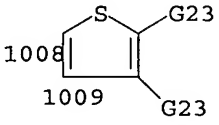


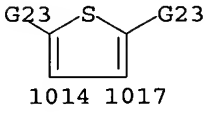
G5 = carbocycle <containing 6 C, non-aromatic,
saturated, 6-membered monocyclic ring> /
heterocycle <containing 1 heteroatom, 1 N, 8 C, aromatic,
6 normalized bonds, 2 C fusion atoms, bicyclic,
(1) 5-membered ring, (1) 6-membered ring> /
heterocycle <containing 1 heteroatom, 1 N, 5 C,
non-aromatic, saturated, 6-membered monocyclic ring> /
993-4 994-831 / 998-4 1002-831 / 1003-4 1006-831 /
1009-4 1008-831 / 1014-4 1017-831 / 1019-4 1021-831 /
phenylene (opt. substd. by G24) / 1026-4 1027-831 /
1032-4 1034-831 / 1038-4 1041-831 / 1050-4 1054-831 /
1057-4 1056-831 / 1063-4 1064-831 / 1069-4 1071-831 /
1075-4 1078-831 / 1080-4 1084-831 / 1086-4 1089-831 /
1109-4 1110-831 / 1115-4 1117-831 / 1121-4 1118-831

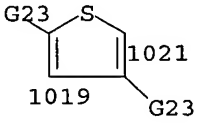


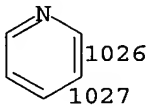


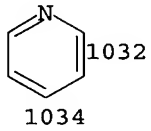


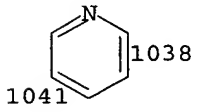


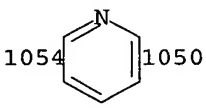


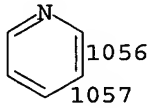


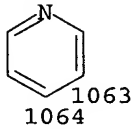


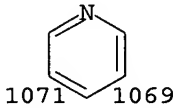


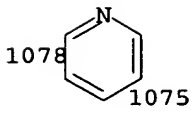


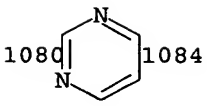


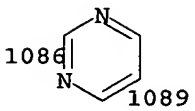


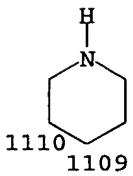


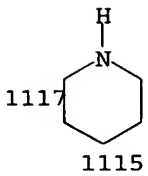




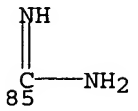


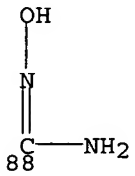


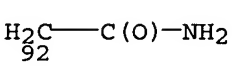


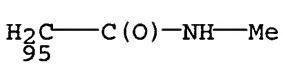


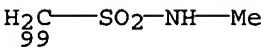
G6 = Et / CH2NH2 / Cl / SO2NH2 / CONH2 / SO2Me / F / Br / Me / OMe / CN
G7 = F / Br / Me
G8 = Cl / H
G9 = H / NH2
G10 = F / Br / Me / Cl
G11 = **C(O)** / CH2
G12 = S(O) / SO2
G13 = H / Cl / F / SO2NH2 / SO2Me / CH2NH2 / CONH2 / CN / 85 / 88 / 92 / 95 / 99 / OMe / 103

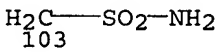




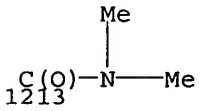


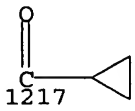


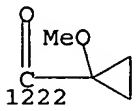




G14 = H / Cl
G15 = H / F / Cl / CONH2 / CH2NH2
G16 = O / S / CH2
G17 = H / Cl
G18 = H / R / (Examples: Me / SO2Me / CO2Me / 1213 / 1217 / 1222 / COMe)

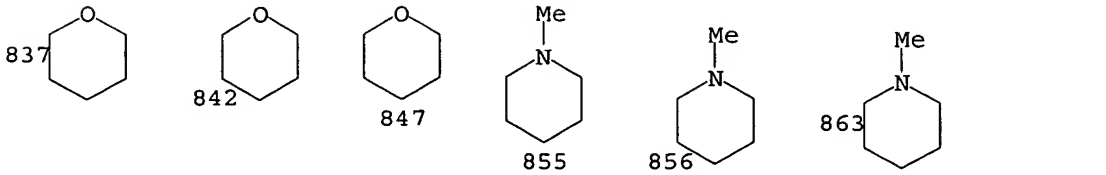


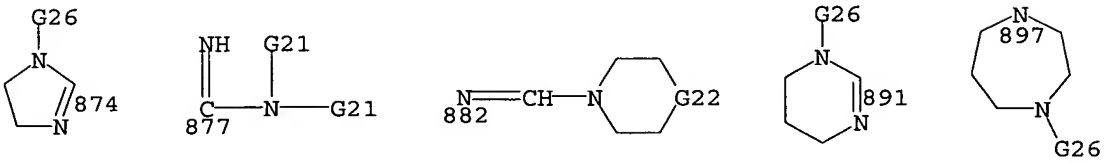


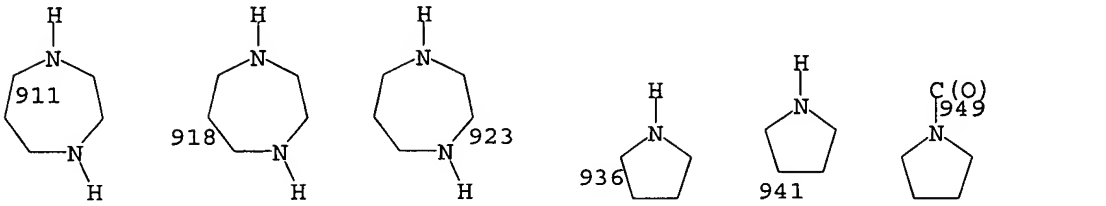


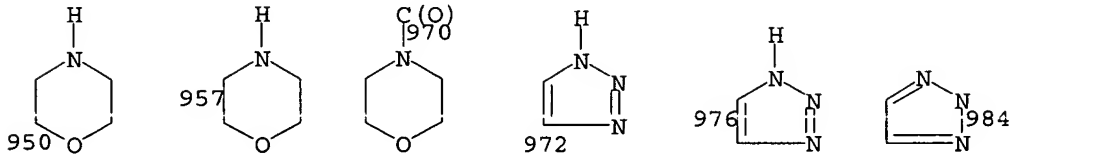
G19 = CH2 / O / NH / SO2
G20 = Pr-i / **cyclopropyl** / cyclobutyl / cyclopentyl / cyclohexyl / 837 / 842 / 847 / 855 / 856 / 863 / pyridyl / 874 / 877 / 882 / 891 / 897 / 911 / 918 / 923 / Ph (opt. substd. by G27) / pyrrolidino / 936 / 941 / 949 / morpholino / 950 / 957 / 970 / 972 / 976 / 984 / 990 /

imidazolyl (opt. substd. by G29) / benzimidazolyl

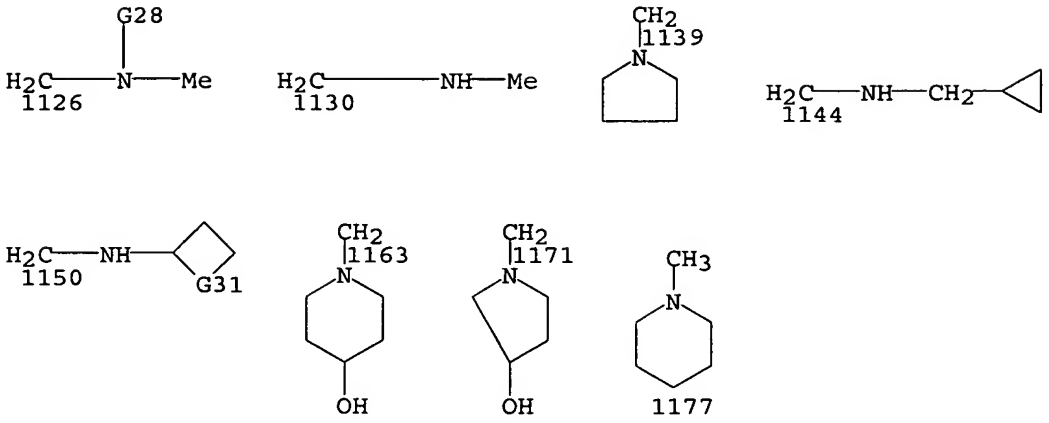




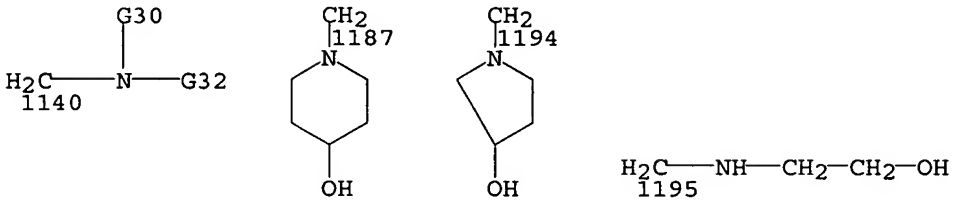




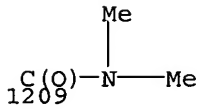
G21 = Me / Et
G22 = bond / CH2 / O
G23 = H / F / Cl
G24 = Cl / F / Me / NH2 / OMe
G25 = any ring <containing 5-6 atoms, 0-1 heteroatom, 0-1 N, 0-1 O, 0-1 S (no other heteroatoms), saturated, 5- to 6-membered monocyclic ring> / any ring <containing 9-10 atoms, 0-2 heteroatoms, 0-2 N, 0-1 O, 0-1 S (no other heteroatoms), attached through 2 or more C, bicyclic, 5- or 6-membered rings only>
G26 = H / (Specifically claimed: Me)
G27 = R / (Specifically claimed: SO2Me / 1126 / 1130 / 1139 / 1144 / 1150 / 1163 / 1171 / 1177)



G28 = Me / Et
G29 = Me / 1140 / 1187 / 1194 / 1195



G30 = H / Me
G31 = (1-2) CH2
G32 = Me / cyclobutyl / cyclopentyl
G33 = H / R / (Examples: CO2Me / CH2OH / NH2)
G34 = H / R / (Examples: 1209 / OMe)



Patent location: claim 1
Note: or pharmaceutically acceptable salts
Note: additional substitution also claimed
Note: substitution is restricted

L29 ANSWER 3 OF 5 MARPAT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 142:336464 MARPAT
TITLE: Preparation of heterocyclic substituted silicon compounds with microbiocidal activity
INVENTOR(S): Ehrenfreund, Josef; Lamberth, Clemens; Tobler, Hans; Walter, Harald
PATENT ASSIGNEE(S): Syngenta Participations Ag, Switz.
SOURCE: PCT Int. Appl., 68 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005028485	A1	20050331	WO 2004-EP10009	20040908
WO 2005028485	C1	20050609		

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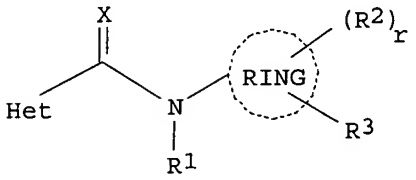
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: GB 2003-22012 20030919

GI

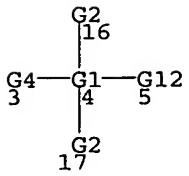


I

AB Preparation of fungicidal compds. I (X = O, S; RING = Ph, thienyl; Het = 5- or 6-membered heterocyclic ring containing one to three heteroatoms, each independently selected from O, N, S, the ring being substituted by one to four groups R4; R1 = H, optionally substituted (C1-4)alkyl, formyl, optionally substituted (C1-4)alkylC(:O), optionally substituted (C1-4)alkylC(:O)O, optionally substituted (C1-4)alkoxy(C1-4)alkyl, optionally substituted allyl, optionally substituted propargyl or optionally substituted allenyl; R2 = independently, halo, optionally substituted (C1-4)alkyl, optionally substituted (C1-4)alkoxy or optionally substituted (C1-4)alkoxy(C1-4)alkyl; R3 = (CRaRb)m-Cy-(CRCRd)n-Y; R4 = independently, selected from halo, C1-3 alkyl, C1-3 haloalkyl, C1-3 alkoxy(C1-3)alkyl and cyano; Ra, Rb, Rc, Rd = independently, H, optionally substituted (C1-4)alkyl; Cy is an optionally substituted carbocyclic or heterocyclic 3-7 membered ring which may be saturated, unsatd. or aromatic and which optionally contains a silicon atom as a ring member; (CRaRb)m and (CRcRd)n may be bound either to the same carbon or silicon atom of Cy or to different atoms separated by 1, 2 or 3 ring members; Y = silyloxy etc.), useful as fungicides in agriculture (activity given), is described. Thus, reaction of N-methyl-3-difluoromethyl-4-chlorocarbonylpyrazole with 1,1-dimethyl-3-(2'-amino)phenylsilacyclohexane (preparation given) gave title compound which was used as fungicides (activity given).

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

MSTR 1



G1 = 23-3 20-5 22-17 21-16 / 29-3 26-5 28-17 24-16 /
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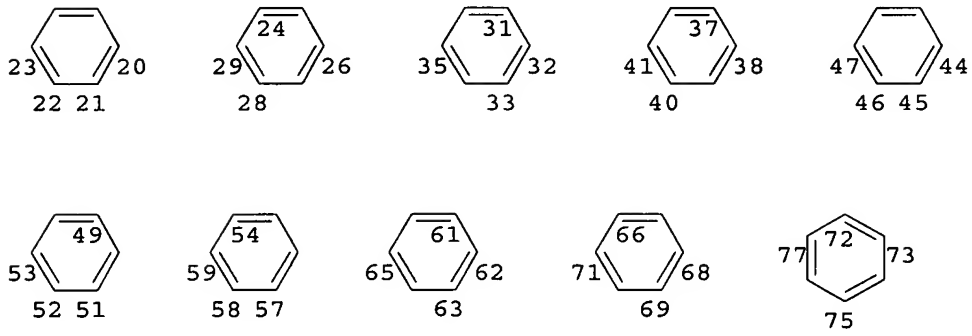
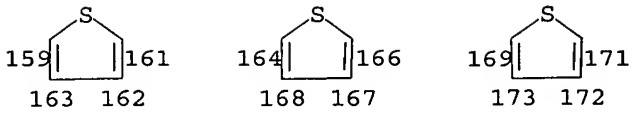
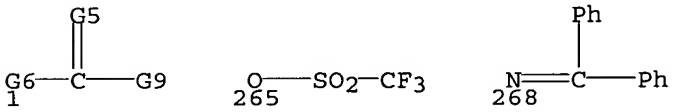
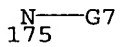




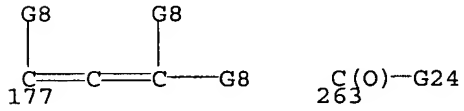
G2 = H / F / Cl / Br / I / alkyl <containing 1-4 C> (opt. substd. by 1 or more G3) / alkoxy <containing 1-4 C> (opt. substd.) / (Specifically claimed: Me / CF3 / OCF3)
G3 = R / alkoxy <containing 1-4 C> (opt. substd.)
G4 = 1 / NH2 / NHCHO / alkylcarbonylamino <containing 1-4 C> (opt. substd.) / alkoxycarbonylamino <containing 1-4 C> (opt. substd.) / Br / I / NO2 / 265 / 268



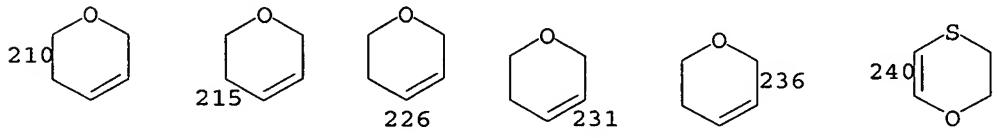
G5 = O / S
G6 = **NH** / 175

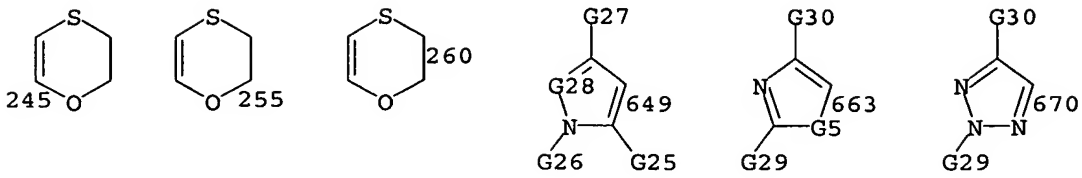


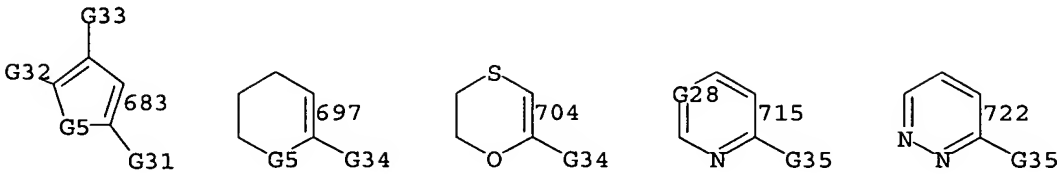
G7 = alkyl <containing 1-4 C> (opt. substd. by 1 or more G3) / CHO / alkylcarbonyl (opt. substd.) / alkylcarbonyloxy (opt. substd.) / CH2CH=CH2 (opt. substd.) / propargyl (opt. substd.) / 177 / (Specifically claimed: 263)

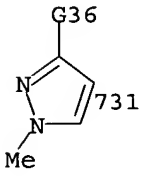


G8 = H / R
G9 = heterocycle <containing 5-6 atoms, 1-3 heteroatoms, zero or more N, zero or more O, zero or more S (no other heteroatoms)> (opt. substd. by (1-4) G10) / (Specifically claimed: pyrazolyl / pyrrolyl / thienyl / furyl / thiazolyl / isothiazolyl / oxazolyl / isoxazolyl / triazolyl / pyridyl / pyrazinyl / pyrimidinyl / pyridazinyl / 210 / 215 / 226 / 231 / 236 / 240 / 245 / 255 / 260) / **(Examples: 649** / 663 / 670 / 683 / 697 / 704 / 715 / 722 / 731)





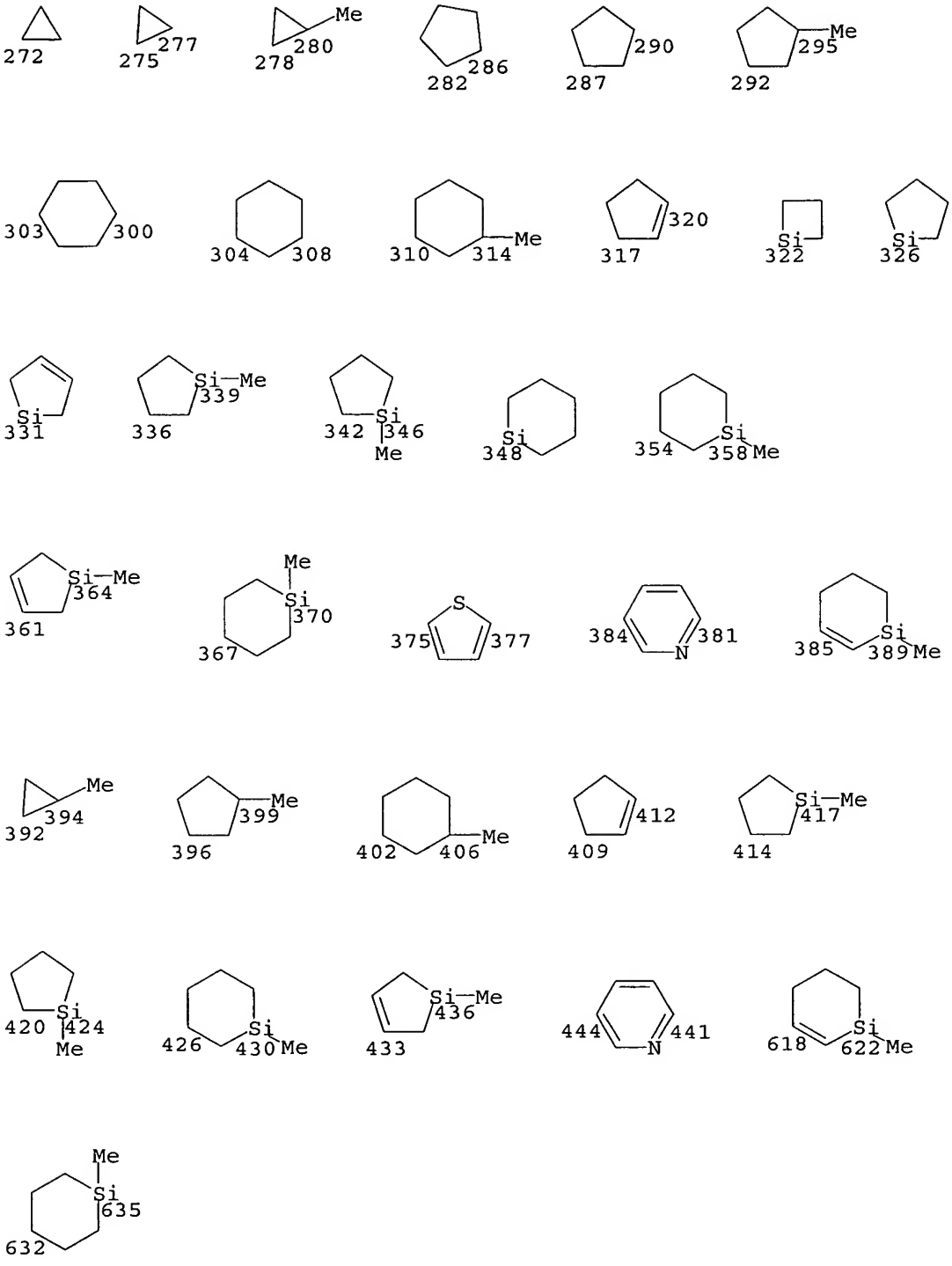




G10 = F / Cl / Br / I / alkyl <containing 1-3 C>
(opt. substd. by alkoxy <containing 1-3 C>) /
alkyl <containing 1-3 C> (substd. by 1 or more G11) / CN
G11 = F / Cl / Br / I
G12 = 7 / 192

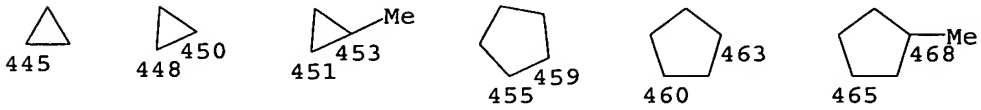
G15—G17 G13—G16—G17
7 8 192 184

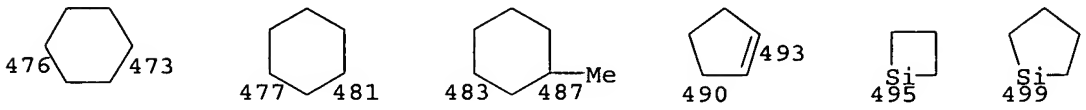
G13 = alkylene <containing 1 or more C> (opt. substd.) /
G14
G14 = (1-3) CH2
G15 = carbocycle <containing 3-7 C,
0 or more double bonds, 0 or more triple bonds,
0 or more normalized bonds> (opt. substd.) /
heterocycle <containing 3-7 atoms, zero or more Si,
0 or more double bonds, 0 or more triple bonds,
0 or more normalized bonds> (opt. substd.) / **(Examples: 272**
/
275-4 277-8 / 278-4 280-8 / 282-4 286-8 / 287-4 290-8 /
292-4 295-8 / 303-4 300-8 / 304-4 308-8 / 310-4 314-8 /
317-4 320-8 / 322 / 326 / 331 / 336-4 339-8 /
342-4 346-8 / 348 / 354-4 358-8 / 361-4 364-8 /
367-4 370-8 / p-C6H4 / m-C6H4 / 375-4 377-8 /
384-4 381-8 / 385-4 389-8 / 394-4 392-8 / 399-4 396-8 /
406-4 402-8 / 412-4 409-8 / 417-4 414-8 / 424-4 420-8 /
430-4 426-8 / 436-4 433-8 / 441-4 444-8 / 622-4 618-8 /
635-4 632-8)

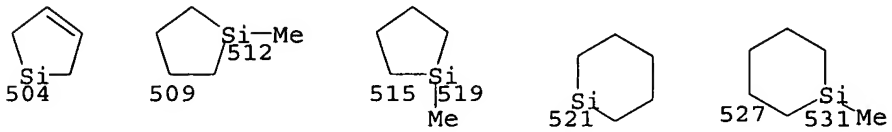


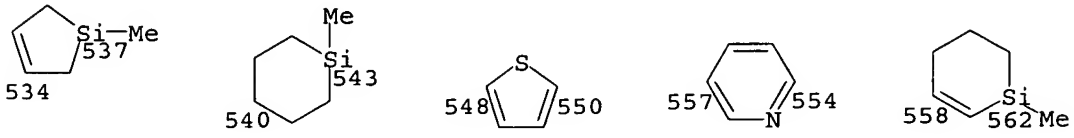
G16 = carbocycle <containing 3-7 C,
0 or more double bonds, 0 or more triple bonds,
0 or more normalized bonds> (opt. substd.) /
heterocycle <containing 3-7 atoms, zero or more Si,
0 or more double bonds, 0 or more triple bonds,
0 or more normalized bonds> (opt. substd.) / (Examples: 445 /

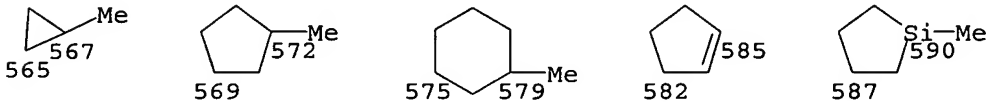
448-192 450-184 / 451-192 453-184 / 455-192 459-184 /
460-192 463-184 / 465-192 468-184 / 476-192 473-184 /
477-192 481-184 / 483-192 487-184 / 490-192 493-184 /
495 / 499 / 504 / 509-192 512-184 / 515-192 519-184 / 521 /
527-192 531-184 / 534-192 537-184 / 540-192 543-184 /
p-C6H4 / m-C6H4 / 548-192 550-184 / 557-192 554-184 /
558-192 562-184 / 567-192 565-184 / 572-192 569-184 /
579-192 575-184 / 585-192 582-184 / 590-192 587-184 /
597-192 593-184 / 603-192 599-184 / 609-192 606-184 /
614-192 617-184 / 629-192 625-184 / 642-192 639-184)

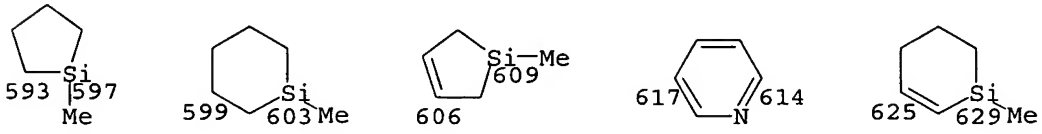


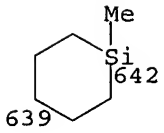




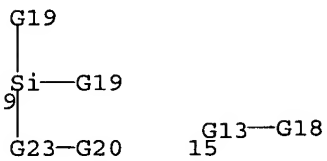




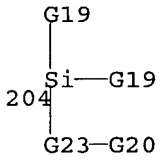




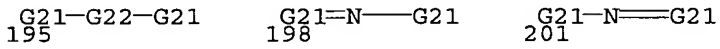
G17 = 15 / H / 9



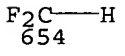
G18 = H / 204



G19 = Me / Et / OMe / OEt
G20 = alkyl <containing 1-4 C>
(opt. substd. by (1-3) G11) / alkenyl <containing 2-4 C>
(opt. substd. by (1-3) G11) / 195 / 198 / 201 /
(Examples: Me / Pr-i / Bu-t / Et)



G21 = carbon chain <containing 1-3 C,
0 or more double bonds, no triple bonds>
(opt. substd. by (up to 3) G11)
G22 = O / S / NH (opt. substd.)
G23 = bond / O
G24 = Me / Et / CH2OMe
G25 = H / **F** / Cl
G26 = Me / CH2OMe / 654



G27 = CF3 / 656 / Me / 658

G28 = **N** / CH
G29 = Me / CH2OMe / CF3
G30 = CF3 / 674 / 676 / Me / 678

F_2C——H (674) F_2C——Cl (676) H_2C——F (678)

G31 = H / Me
G32 = Me / H
G33 = CF3 / 688 / 690 / Me / H / 692

F_2C——H (688) F_2C——Cl (690) H_2C——F (692)

G34 = CF3 / Me / 708 / 710

F_2C——Cl (708) F_2C——H (710)

G35 = CF3 / Cl / 726

F_2C——Cl (726)

G36 = CF3 / 735

F_2C——H (735)

Patent location: claim 1
Note: or N-oxides, geometric isomers, tautomers, or isotopic forms
Note: substitution is restricted
Note: also incorporates claim 8, structure II
Stereochemistry: or optical isomers

L29 ANSWER 4 OF 5 MARPAT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 140:235719 MARPAT
TITLE: Preparation of triazolylcarboxylic acid derivatives with antifungal activity for agricultural use
INVENTOR(S): Ehrenfreund, Josef; Tobler, Hans; Walter, Harald
PATENT ASSIGNEE(S): Syngenta Participations A.-G., Switz.
SOURCE: PCT Int. Appl., 82 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

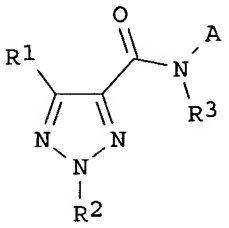
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004018438	A2	20040304	WO 2003-EP9111	20030818
WO 2004018438	A3	20040826		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM,

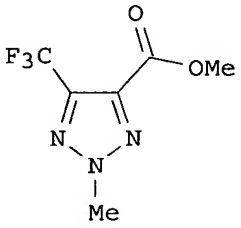
PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN,
TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

CA 2494263	AA	20040304	CA 2003-2494263	20030818	
AU 2003253417	A1	20040311	AU 2003-253417	20030818	
EP 1539717	A2	20050615	EP 2003-792351	20030818	
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK					
BR 2003013686	A	20050621	BR 2003-13686	20030818	
CN 1678593	A	20051005	CN 2003-819890	20030818	
JP 2006502244	T2	20060119	JP 2005-501204	20030818	
PRIORITY APPLN. INFO.:			GB 2002-19612	20020822	
			GB 2003-10464	20030507	
			WO 2003-EP9111	20030818	

GI



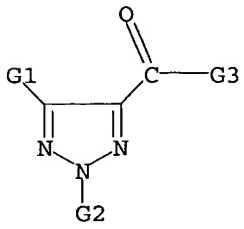
I



II

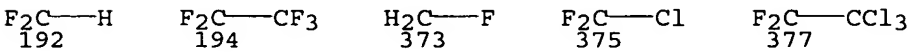
AB Title compds. I [A = ortho-substituted aryl or heteroaryl ring system; R1 = halo, CN, NO2, alkyl, haloalkyl, alkoxy, haloalkoxy, (un)substituted alkene, etc.; R2 = alkyl, haloalkyl, alkoxyalkyl, etc.; R3 = H, (un)substituted-alkyl, -propargyl, -alkoxy, etc.] were prepared and disclosed as having antifungal activity. Thus, e.g., II was prepared via methylation of 1,2,3-triazole-4,5-dicarboxylic acid di-Me ester, with subsequent monohydrolysis and fluorination of the carboxylic acid moiety to the trifluoromethyl moiety. I were tested against 9 different agriculturally relevant fungi with varying degrees of efficacy observed Addnl., a composition of I with a suitable carrier for controlling microorganisms and preventing attack and infestation of plants therewith is claimed.

MSTR 1

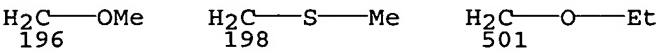


G1 = F / Cl / Br / I / **CN** / NO2 /

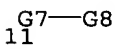
alkyl <containing 1-4 C> (opt. substd. by 1 or more G11) /
alkoxy <containing 1-4 C> (opt. substd. by 1 or more G11) /
alkenyl <containing 2-4 C> (opt. substd. by 1 or more G12) /
alkynyl <containing 2-4 C> (opt. substd. by 1 or more G12) /
alkylsulfonyl <containing 1-4 C>
(opt. substd. by 1 or more G12) /
(Specifically claimed: OCF3) / (Examples: 192 / CF3 / CH3 /
194 / 373 / 375 / Et / 377)



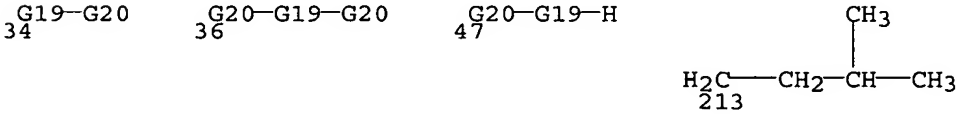
G2 = alkyl <containing 1-4 C>
(opt. substd. by (1-3) G13) / (Examples: Me / Et / 196 /
198 / 501)

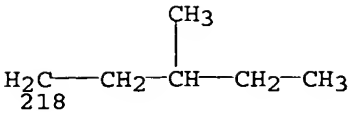


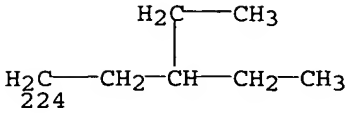
G3 = **11** / F / Cl / Br / I / OH /
alkoxy <containing 1-5 C> / (Examples: OMe / OEt / OPr-n /
OPr-i)

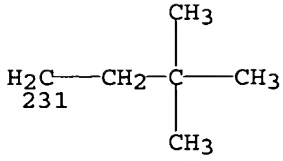


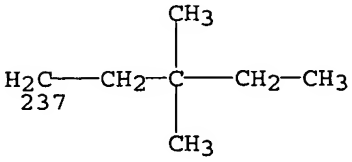
G4 = H / F / Cl / Br / I / alkyl <containing 1-4 C>
(opt. substd. by 1 or more G11) /
alkoxy <containing 1-4 C> (opt. substd. by 1 or more G11)
G5 = H / alkyl <containing 1-6 C>
(opt. substd. by 1 or more G15) /
alkoxy <containing 1-4 C> (opt. substd. by 1 or more G15) /
alkyl <containing 1-4 C> (opt. substd. by 1 or more G16) /
aryl (opt. substd. by 1 or more G15)
G6 = Ph (opt. substd. by G37) /
heterocycle <containing 5-6 atoms, 1-3 heteroatoms,
zero or more N, zero or more O,
zero or more S (no other heteroatoms), monocyclic> /
alkyl <containing 3-12 C> (opt. substd.) /
alkenyl <containing 2-12 C> (opt. substd.) /
alkynyl <containing 2-12 C> / cycloalkyl <containing 3-8 C> /
cycloalkenyl <containing 4-8 C> /
cycloalkyl <containing 6-12 C, bicyclic> / 34 / 36 / 47 /
(Examples: Pr-n / Bu-n / pentyl / 213 / 218 / 224 / 231 /
237 / 244 / 248 / 253 / 257 / 262 / 268 / 275 / 283 / 290 /
298 / 303 / 310 / 316 / cycloheptyl /
thienyl (opt. substd. by Cl) / furyl (opt. substd. by Cl) /
pyridyl / 3-pyridyl (substd. by G42) / 322 / 328 / Pr-i /
SiMe3 / 332 / 342 / 343 / 362 / 491)

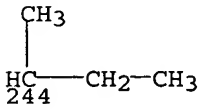


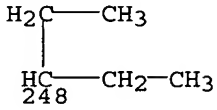

CH3
H2C—CH2—CH—CH2—CH3
218

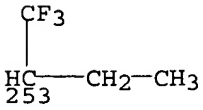

H2C—CH3
H2C—CH2—CH—CH2—CH3
224

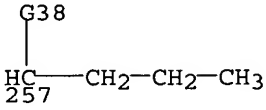

CH3
H2C—CH2—C—CH3
231
CH3

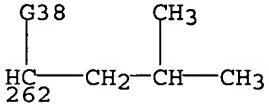

CH3
H2C—CH2—C—CH2—CH3
237
CH3

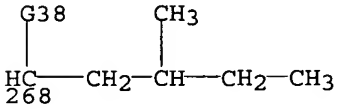

CH3
HC—CH2—CH3
244

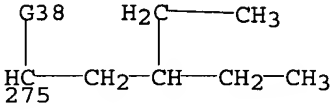

H2C—CH3
HC—CH2—CH3
248

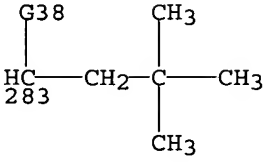

CF3
HC—CH2—CH3
253

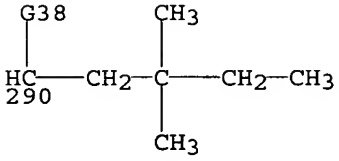

G38
HC—CH2—CH2—CH3
257

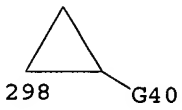

G38
CH3
HC—CH2—CH—CH3
262

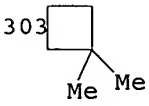

G38
CH3
HC—CH2—CH—CH2—CH3
268

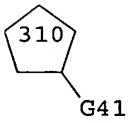

G38
H2C—CH3
HC—CH2—CH—CH2—CH3
275

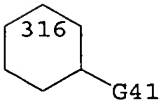

G38
CH3
HC—CH2—C—CH3
283
CH3

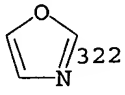

G38
CH3
HC—CH2—C—CH2—CH3
290
CH3

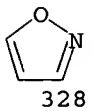

298
G40

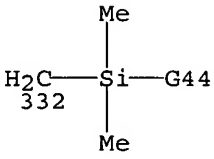

303
Me
Me

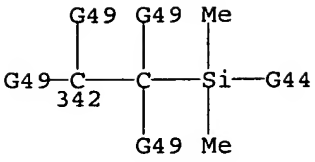

310
G41

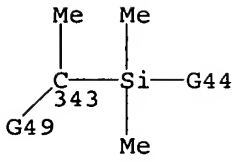

316
G41

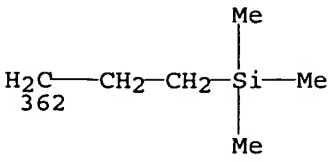

O
322
N

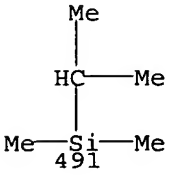

O
N
328


Me
H2C—Si—G44
332
Me

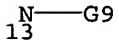




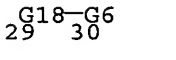


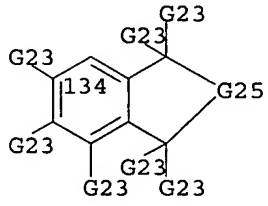


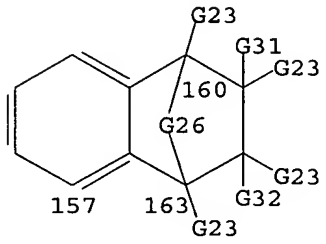
G7 = **NH** / 13

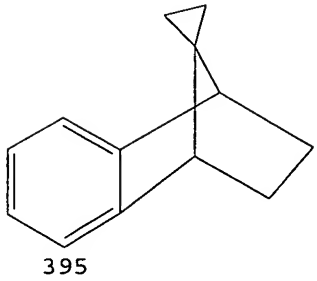


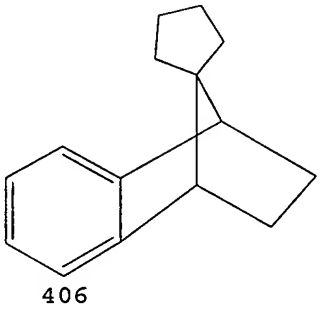
G8 = **29** / 1-naphthyl (opt. substd. by 1 or more G23) / 134 / 157 / (Examples: 395 / 406 / 417 / 448 / 462 / 478)

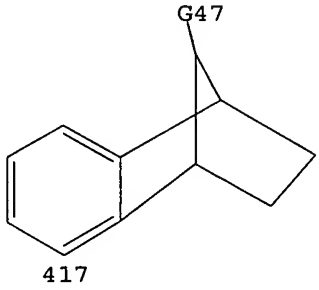


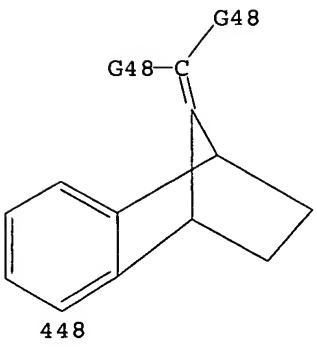




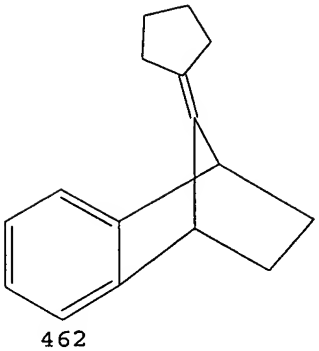








448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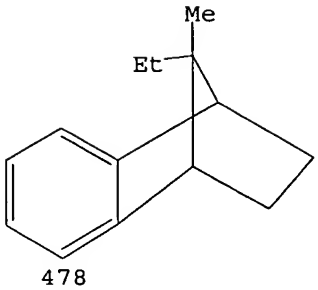
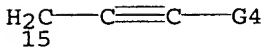
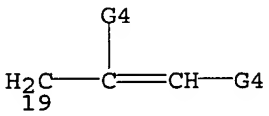


478

G9 = 15 / 19 / 24 / 27 / alkyl <containing 1-4 C> (opt. substd. by (1-3) G17) / alkoxy <containing 1-4 C> (opt. substd. by (1-3) G17) / alkylcarbonyloxy <containing 1-4 C> (opt. substd. by (1-3) G17) / (Examples: COMe / 201 / CO2Bu-t)


15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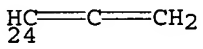
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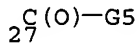
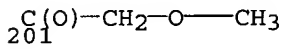
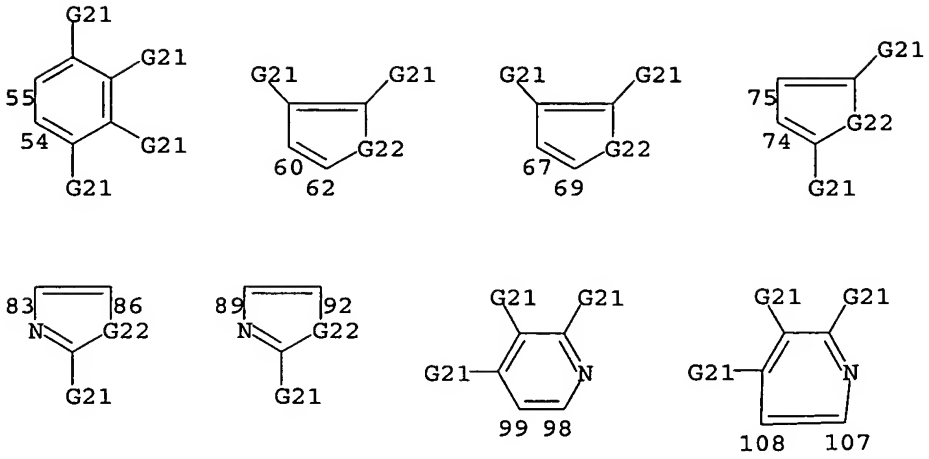
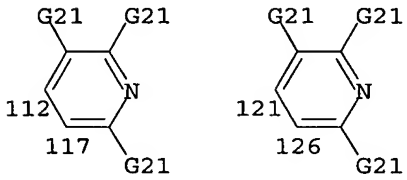

27

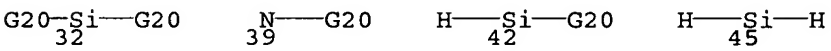

201

G11 = F / Cl / Br / I
G12 = F / Cl / Br / I / alkoxy <containing 1-4 C>
G13 = F / Cl / Br / I / alkoxy <containing 1-4 C> / alkylthio <containing 1-4 C> / aryl (opt. substd. by (1-3) G14) / aryloxy (opt. substd. by (1-3) G14)
G14 = F / Cl / Br / I / alkoxy <containing 1-4 C>
G15 = F / Cl / Br / I / alkoxy <containing 1-6 C> (opt. substd. by 1 or more G11) / CN / OH / CO2Me / CO2Et
G16 = F / Cl / Br / I / alkoxy <containing 1-6 C> (opt. substd. by 1 or more G11) / CN / OH / CO2Me / CO2Et / alkoxy <containing 1-4 C> (opt. substd. by 1 or more G15) / alkylthio <containing 1-4 C> (opt. substd. by 1 or more G15)
G17 = F / Cl / Br / I / alkoxy <containing 1-4 C> / alkyl <containing 1-4 C> / alkoxy <containing 1-2 C> (substd. by 1 or more G11) / OH / CN / CO2H / CO2Me / CO2Et / SO2Me / SO2Et
G18 = 55-11 54-30 / **60-11 62-30** / 69-11 67-30 / 75-11 74-30 / 83-11 86-30 / 92-11 89-30 / 99-11 98-30 / 107-11 108-30 / 112-11 117-30 / 126-11 121-30

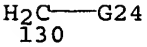




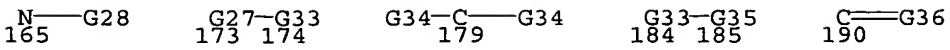
G19 = O / S / 32 / NH / 39 / 42 / 45



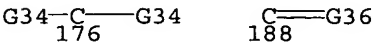
G20 = carbon chain <containing up to 13 C> (opt. substd.) / carbocycle <containing 3-13 C> (opt. substd.)
G21 = H / F / Cl / Br / I / CN / NO2 / alkyl <containing 1-4 C> (opt. substd. by 1 or more G11) / alkoxy (opt. substd. by 1 or more G11) / alkylthio <containing 1-4 C> (opt. substd. by 1 or more G11) / (Example: Me)
G22 = O / **S**
G23 = H / F / Cl / Br / I / alkyl <containing 1-4 C> (opt. substd. by 1 or more G11) / COMe / alkoxy <containing 1-4 C> (opt. substd. by 1 or more G11) / alkylthio <containing 1-4 C> (opt. substd. by 1 or more G11) / CH2OH / 130 / (Examples: Me / OMe / CF3 / Et)



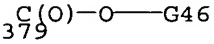
G24 = alkoxy <containing 1 or more C>
G25 = CH2CH2 / CH2CH2CH2 / CH2 / O / S
G26 = O / 165 / S / 173-160 174-163 / 179 / 190 / 184-160 185-163 / cycloalkylene <containing 3-5 C, attached through 1 C>



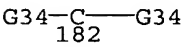
G27 = 188 / 176 / cycloalkylene <containing 3-5 C, attached through 1 C>



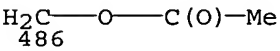
G28 = H / alkyl <containing 1-4 C> (opt. substd. by alkoxy <containing 1-4 C>) / CHO / alkylcarbonyl <containing 1-4 C> (opt. substd. by 1 or more G29) / alkoxycarbonyl <containing 1-6 C> (opt. substd. by 1 or more G30) / (Examples: Me / COMe / 379)



G29 = F / Cl / Br / I / alkoxy <containing 1-4 C>
G30 = F / Cl / Br / I / alkoxy / CN
G31 = H
G32 = H
G33 = (1-2) 182

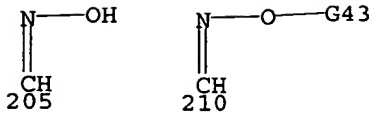


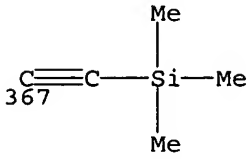
G34 = H / alkyl <containing 1-6 C> (opt. substd.) / alkenyl <containing 2-6 C> (opt. substd.) / carbocycle <containing 3-7 C> (opt. substd.) / F / Cl / Br / I / OH / alkoxy <containing 1-4 C> / (Examples: Me / Et / OMe / 486 / CH2Ph / OPr-n / CH2OH / CHO)



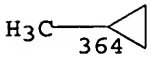
G35 = 186 / cycloalkylene <containing 3-5 C, attached through 1 C>

G36 = O / cycloalkylene <containing 3-6 C> / carbon chain <containing 1-9 C, saturated>
G37 = R / (Examples: F / Cl / I / Br / CF3 / OCF3 / SCF3 / 205 / 210 / CN / NO2 / ethynyl / 367 / CH=CH2)

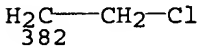




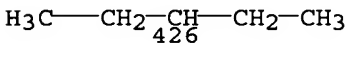
G38 = Me / Et / CF3
G40 = Bu-t / Bu-i / cyclopropyl / 364 / cyclobutyl / cyclopentyl / cyclohexyl

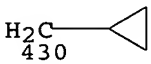


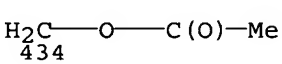
G41 = H / Me
G42 = F / Cl / Br
G43 = Me / Bu-n / Bu-i / Pr-i / Pr-n / Et
G44 = Me / Et / Pr-i / OMe
G46 = Me / Et / Bu-i / Bu-n / Bu-t / 382



G47 = H / Pr-n / 426 / 430 / cyclopentyl / Et / OPr-i / CH2Ph / Pr-n / 434







G48 = Me / Et
G49 = H / Me
G31+G32= bond
Patent location: claim 1
Note: substitution is restricted
Note: also incorporates claim 6

L29 ANSWER 5 OF 5 MARPAT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 139:365221 MARPAT
TITLE: Preparation of amino acid derivatives as antidiabetic agents
INVENTOR(S): Maruta, Katsunori; Nagata, Ryu; Iwai, Kiyotaka; Ushiroda, Kantaro; Yoshida, Kozo
PATENT ASSIGNEE(S): Sumitomo Pharmaceuticals Co., Ltd., Japan
SOURCE: PCT Int. Appl., 207 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

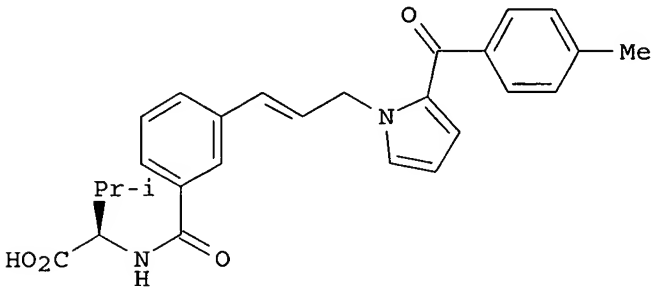
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003091211	A1	20031106	WO 2003-JP3935	20030328

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,

CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM,
PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT,
TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2003220896 A1 20031110 AU 2003-220896 20030328
PRIORITY APPLN. INFO.: JP 2002-90206 20020328
WO 2003-JP3935 20030328

GI



I

AB The title compds. with general formula of R1-X1-Ar1-W1-Z-W2-Ar2 [wherein ring Z = (un)substituted pyrrole, pyrazole, imidazole, triazole, indole, indazole, or benzimidazole; W2 = a single bond, SO, SO2, (un)substituted CONH, SO2NH, alkylene, alkenylene, or alkynylene; Ar2 = (un)substituted aryl or heteroaryl; W1 = (un)substituted alkylene, alkenylene, alkynylene, or Y-W3, etc.; Y = O, S, or (un)substituted NH; W3 = (un)substituted alkylene, alkenylene, or alkynylene; Ar1 = (un)substituted arylene or heteroarylene; X1 = SO2, OCO2, SO3, (un)substituted CONHSO2, NHSO2, NHCO, SO2NHCO, SO2NH, CONH, OCONH, NHCONH, -NH-C(NH2)=N-, NHCO2, or Y2-W4; Y2 = S, (un)substituted NHCO, CONH, CH=NO, NH, -N(CO2H)-, -N(COH)-, -N(SO2H)-, or -N(CONH2)-; W4 = (un)substituted alkylene; R1 = (un)substituted alkyl, alkoxy, alkenyl, or alkynyl, etc.] and prodrugs or pharmaceutically acceptable salts thereof are prepared The title compds. have an effect of activating PPARα, PPARγ, or controlling the activation of PPARα/γ, and improve insulin resistance, and are useful for the treatment of diabetes (no data). For example, the compound I was prepared in a multi-step synthesis. I showed agonist activities of 20.2 and 4.2 at the concentration of 10 μM against human PPARα and PPARγ, resp.

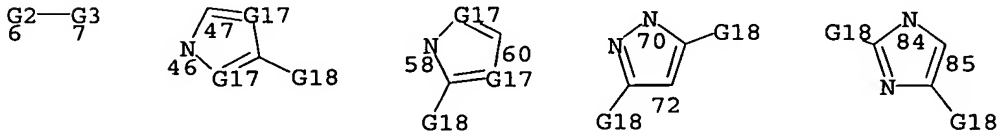
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

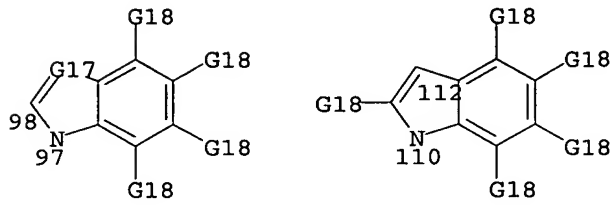
MSTR 1

G16—G14—G9—G1—G8
1 2 3 4 5

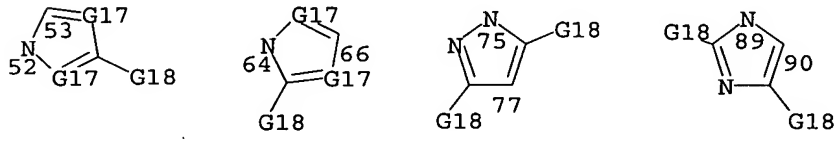
G1 = heterocycle <containing 5 atoms, 1-3 heteroatoms, 1-3 N (no other heteroatoms), aromatic, 2 double bonds, 5-membered monocyclic ring> (opt. substd.) / heterocycle <containing 9 atoms, 1-2 heteroatoms,

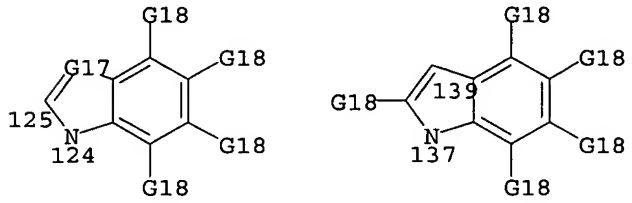
1-2 N (no other heteroatoms), aromatic, 6 normalized bonds,
1 double bond, bicyclic, (1) 5-membered ring,
(1) 6-membered ring> (opt. substd.) / 6-3 7-5 /
(Specifically claimed: 46-3 47-5 / 58-3 60-5 / 70-3 72-5 /
84-3 85-5 / 97-3 98-5 / 110-3 112-5)



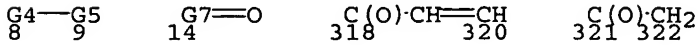


G2 = heterocycle <containing 5 atoms, 1-3 heteroatoms,
1-3 N (no other heteroatoms), aromatic, 2 double bonds,
5-membered monocyclic ring> (opt. substd.) /
heterocycle <containing 9 atoms, 1-2 heteroatoms,
1-2 N (no other heteroatoms), aromatic, 6 normalized bonds,
1 double bond, bicyclic, (1) 5-membered ring,
(1) 6-membered ring> (opt. substd.) /
(Specifically claimed: 52-3 53-7 / 64-3 66-7 / 75-3 77-7 /
89-3 90-7 / 124-3 125-7 / 137-3 139-7)

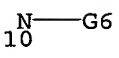




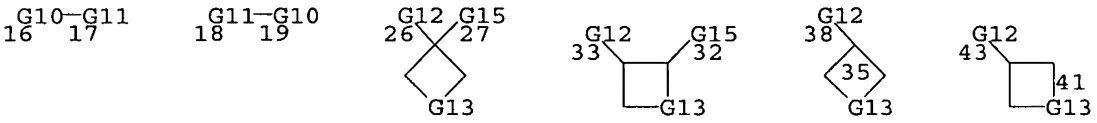
G3 = S(O) / SO2 / 8-6 9-5 /
alkylene <containing 1-4 C> (opt. substd.) /
alkenylene <containing 2-4 C> (opt. substd.) /
alkynylene <containing 2-4 C> (opt. substd.) / 14 /
(Examples: C(O) / 318-6 320-5 / 321-6 322-5)

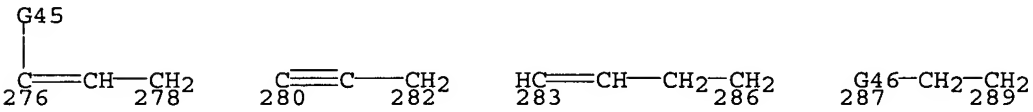


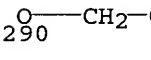
G4 = C(O) / SO2
G5 = NH / 10



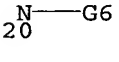
G6 = alkyl (SO aryl (opt. substd. by))
G7 = carbon chain <containing 1-4 C,
0 or more double bonds, 0 or more triple bonds>
(opt. substd.)
G8 = aryl (opt. substd.) / heteroaryl (opt. substd.) /
(Specifically claimed: p-C6H4Me) /
(Examples: Ph (opt. substd.) / thienyl (opt. substd.) /
furyl (opt. substd.) / pyrrolyl (opt. substd.) /
pyridyl (opt. substd.) / pyrimidinyl (opt. substd.) /
indolyl (opt. substd.) / benzothiazolyl (opt. substd.) /
benzoxazolyl (opt. substd.) / benzofuranyl (opt. substd.) /
benzothienyl (opt. substd.))
G9 = alkylene <containing 1-5 C> (opt. substd.) /
alkenylene <containing 2-5 C> (opt. substd.) /
alkynylene <containing 2-5 C> (opt. substd.) / 16-2 17-4 /
18-2 19-4 / **38-2 35-4** / 26-2 27-4 / 43-2 41-4 /
33-2 32-4 / (Examples: 276-2 278-4 / 280-2 282-4 /
283-2 286-4 / CH2CH2 / 287-2 289-4 / 290-2 293-4 /
CH2CH2CH2)





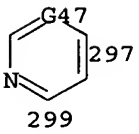


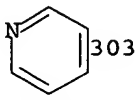
G10 = alkylene <containing 1-4 C> (opt. substd.) /
alkenylene <containing 2-4 C> (opt. substd.) /
alkynylene <containing 2-4 C> (opt. substd.)
G11 = O / S / NH / 20

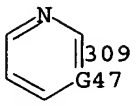


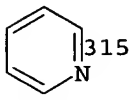
G12 = **(0-3) CH2**
G13 = **(0-2) CH2**
G14 = arylene (opt. substd.) /
heteroarylene (opt. substd.) / (Examples: m-C6H4 (opt.
substd.) / p-C6H4 (opt. substd.) / 299-1 297-3 /
305-1 303-3 / 311-1 309-3 / 317-1 315-3 / 325-1 329-3 /

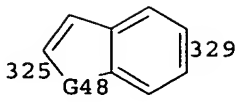
337-1 335-3 / 342-1 340-3)

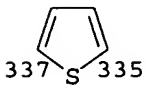


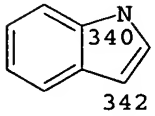




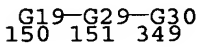


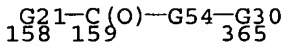


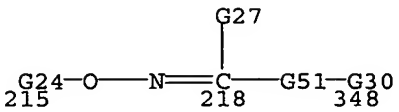


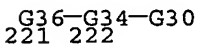


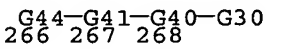
G15 = (1-3) CH2
G16 = **150** / 158 / 215 / **221** / **266** / (Examples: 391 / 444)

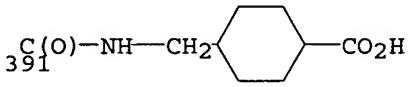


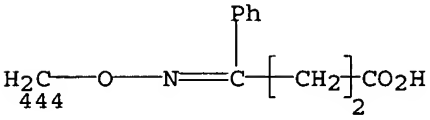




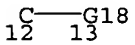




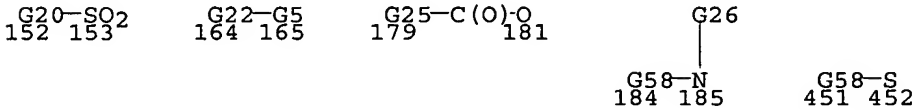




G17 = 12 / N

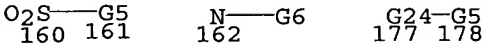


G18 = H / halo / alkyl (opt. substd.) / alkoxy (opt. substd.) / aryl (opt. substd.) / heteroaryl (opt. substd.)
G19 = 152-2 153-151 / 164-2 165-151 / 179-2 181-151 / 184-2 185-151 / 451-2 452-151

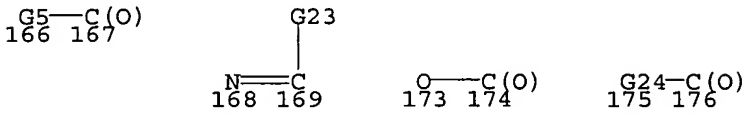


G20 = bond / 156-2 157-153 / NH / 154 / O

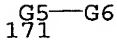
G21 = 160-2 161-159 / NH / 162 / 177-2 178-159



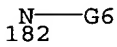
G22 = SO2 / C(O) / 166-2 167-165 / 168-2 169-165 / 173-2 174-165 / 175-2 176-165



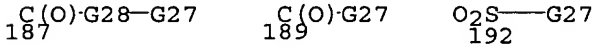
G23 = NH2 / 171



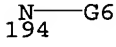
G24 = alkylene <containing 1-4 C> (opt. substd.)
G25 = NH / 182 / O



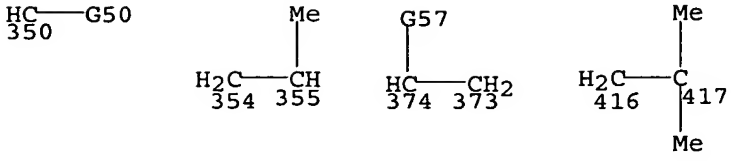
G26 = alkyl (SO aryl (opt. substd. by)) / aryl (opt. substd.) / heteroaryl (opt. substd.) / 187 / 189 / 192



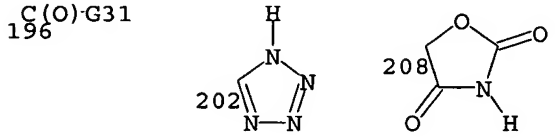
G27 = alkyl (SO aryl (opt. substd. by)) / aryl (opt. substd.) / heteroaryl (opt. substd.)
G28 = O / NH / 194



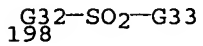
G29 = carbon chain <containing 1 or more C, 0 or more double bonds, 0 or more triple bonds> (substd. by 1 or more G53) / (Examples: 350 / 354-150 355-349 / CH2CH2 / 374-150 373-349 / CMe2 / CH2CH2CH2 / 416-150 417-349)



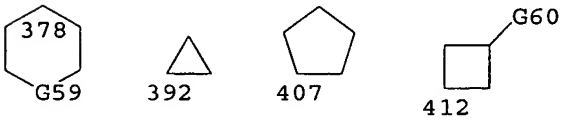
G30 = 196 / 202 / 208 / **CN**



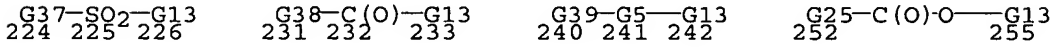
G31 = OH / alkoxy / NH2 (opt. substd.) /
heterocycle <containing 1 or more heteroatoms, 1 or more N, attached through 1 or more N> (opt. substd.) / 198

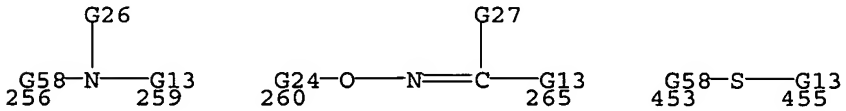


G32 = NH (opt. substd.)
G33 = alkyl (opt. substd.) / aryl (opt. substd.) / heteroaryl (opt. substd.)
G34 = any ring <containing 3-10 atoms, 0-1 heteroatom, 0-1 N, 0-1 O (no other heteroatoms), non-aromatic, saturated, 3- to 10-membered monocyclic ring> (opt. substd. by 1 or more G35) / (**Examples: 378** / 392 / 407 / 412)



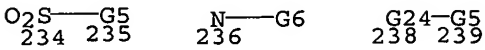
G35 = OH / alkyl / alkoxy / alkylamino / R
G36 = 224-2 226-222 / **231-2 233-222** / 240-2 242-222 / 252-2 255-222 / 256-2 259-222 / 260-2 265-222 / 453-2 455-222



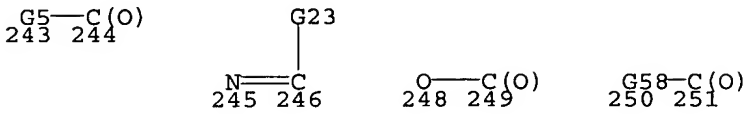


G37 = bond / 227-2 228-225 / NH / 229 / O

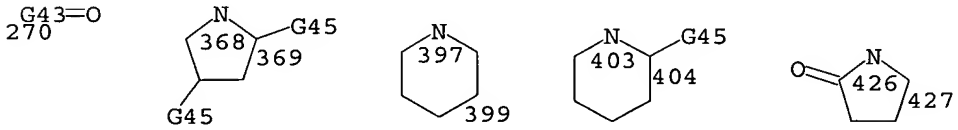
G38 = 234-2 235-232 / **NH** / 236 / 238-2 239-232

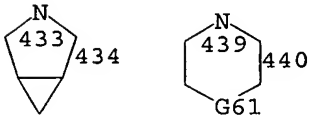


G39 = SO2 / C(O) / 243-2 244-241 / 245-2 246-241 /
248-2 249-241 / 250-2 251-241

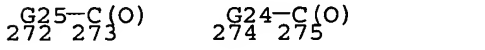


G40 = bond / alkylene <containing 1-4 C> (opt. substd.)
G41 = heterocycle <containing 1-2 heteroatoms,
1 or more N, zero or more O (no other heteroatoms),
attached through 1 or more N, 4- to 10-membered monocyclic
ring> (opt. substd. by G42) / 270 /
(Examples: 368-266 369-268 / 397-266 399-268 /
403-266 404-268 / 426-266 427-268 / 433-266 434-268 /
439-266 440-268)

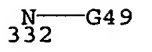




G42 = alkyl <containing 1-4 C> (opt. substd.) / R
G43 = heterocycle <containing 1-2 heteroatoms,
1 or more N, zero or more O (no other heteroatoms),
attached through 1 or more N, 4- to 10-membered monocyclic
ring> (opt. substd. by G42)
G44 = SO2 / C(O) / 272-2 273-267 /
alkylene <containing 1-4 C> (opt. substd.) / 274-2 275-267 /
(Example: CH2)

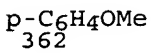


G45 = H / Me
G46 = NH / NMe / O / S
G47 = CH / N
G48 = O / 332

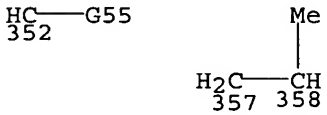


G49 = H / CH2Ph
G50 = Pr-i / 360 / H / Bu-s / CH(OH)Me / CH2CH2SMe / Bu-i / Et / 371 / 2-thienyl

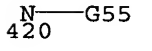
G51 = carbon chain <containing 1 or more C, 0 or more double bonds, 0 or more triple bonds> (substd. by 1 or more G53)
G52 = H / cyclohexyl / 362 / OMe / Ph / OBu-t / OH



G53 = halo / alkoxy (opt. substd. by 1 or more halo) / R
G54 = carbon chain <containing 1 or more C, 0 or more double bonds, 0 or more triple bonds> (substd. by 1 or more G53) / (Examples: 357-159 358-365 / 352)



G55 = H / Me
G56 = F / H
G57 = Ph / Me
G58 = alkylene <containing 1-4 C> (opt. substd.) / (Example: CH2)
G59 = CH2 / **420** / O



G60 = H / OH
G61 = NMe / O
Patent location: claim 1
Note: or pharmacologically acceptable salts

Broader structure search

```
=> file caplus
FILE 'CAPLUS' ENTERED AT 15:21:34 ON 21 MAR 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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FILE LAST UPDATED: 20 Mar 2006  (20060320/ED)

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'OBI' IS DEFAULT SEARCH FIELD FOR 'CAPLUS' FILE

=> d que nos L18
L1              STR
L3       546562 SEA FILE=REGISTRY ABB=ON  PLU=ON  SC4/ES
L5         2304 SEA FILE=REGISTRY SUB=L3 SSS FUL L1
L6              STR
L8              STR
L10         630 SEA FILE=REGISTRY SUB=L5 SSS FUL L8
L15        1135 SEA FILE=REGISTRY SUB=L5 SSS FUL L6
L17         505 SEA FILE=REGISTRY ABB=ON  PLU=ON  L15 NOT L10
L18          22 SEA FILE=CAPLUS ABB=ON  PLU=ON  L17


=> d ibib abs hitstr L18 1-22

L18  ANSWER 1 OF 22  CAPLUS  COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER:         2005:405320  CAPLUS
DOCUMENT NUMBER:          142:425351
TITLE:                    Synergistic fungicidal combinations comprising a
                          carboxamide derivative
INVENTOR(S):              Wachendorff-Neumann, Ulrike; Dahmen, Peter; Dunkel,
                          Ralf; Elbe, Hans-Ludwig; Rieck, Heiko; Suty-Heinze,
                          Anne
PATENT ASSIGNEE(S):       Bayer Cropscience Aktiengesellschaft, Germany
SOURCE:                   PCT Int. Appl., 126 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 German
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.           KIND   DATE        APPLICATION NO.         DATE
     ---------------      ----   --------    --------------------    --------
     WO 2005041653         A2    20050512    WO 2004-EP11403         20041012
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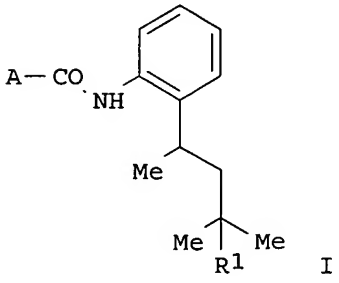
WO 2005041653 A3 20050728
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
DE 10349501 A1 20050525 DE 2003-10349501 20031023
PRIORITY APPLN. INFO.: DE 2003-10349501 A 20031023
OTHER SOURCE(S): MARPAT 142:425351
GI



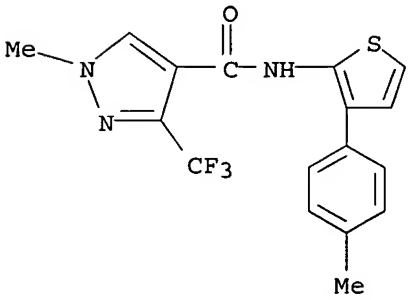
I

AB Synergistic fungicidal combinations comprise a carboxamide derivative I [R1 = H, halo or (halo)alkyl; R1 = (un)substituted Ph, furyl, pyridinyl, etc.] and any of a very large number of known fungicides.

IT **183676-44-0D**, mixture with carboxamide derivative
RL: AGR (Agricultural use); BIOL (Biological study); USES (Uses)
(synergistic fungicidal composition)

RN 183676-44-0 CAPLUS

CN 1H-Pyrazole-4-carboxamide, 1-methyl-N-[3-(4-methylphenyl)-2-thienyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

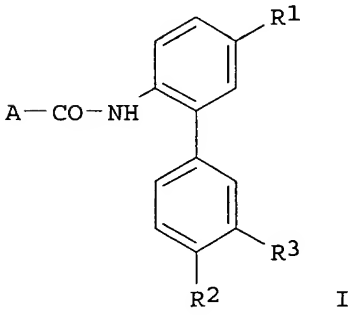


L18 ANSWER 2 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:346774 CAPLUS
DOCUMENT NUMBER: 142:387616
TITLE: Synergistic fungicidal combinations comprising

carboxamide derivatives
INVENTOR(S): Wachendorff-Neumann, Ulrike; Dahmen, Peter; Dunkel, Ralf; Elbe, Hans-Ludwig; Suty-Heinze, Anne; Rieck, Heiko
PATENT ASSIGNEE(S): Bayer Cropscience Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 141 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005034628	A1	20050421	WO 2004-EP10830	20040928
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10347090	A1	20050504	DE 2003-10347090	20031010
PRIORITY APPLN. INFO.:			DE 2003-10347090 A	20031010

OTHER SOURCE(S): MARPAT 142:387616
GI



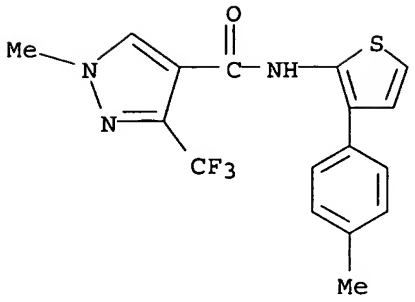
I

AB Synergistic fungicidal mixts. comprise a carboxamide derivative I [R1= H or F; R2 = halo, (halo)alkyl or (halo)alkoxy; , R3 = H, halo or (halo)alkyl; A = (un)substituted Ph, imidazolyl, thiazolyl, etc.] and any of 22 groups of known fungicides.

IT **183676-44-0D**, mixture with carboxamide derivative
RL: AGR (Agricultural use); BIOL (Biological study); USES (Uses)
(synergistic fungicidal combination)

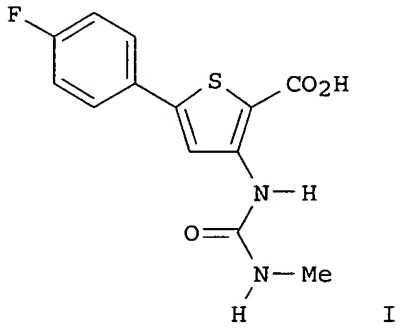
RN 183676-44-0 CAPLUS

CN 1H-Pyrazole-4-carboxamide, 1-methyl-N-[3-(4-methylphenyl)-2-thienyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:41342 CAPLUS
DOCUMENT NUMBER: 142:261352
TITLE: Solution-phase parallel synthesis of a 1140-member ureidothiophene carboxylic acid library
AUTHOR(S): Le Foulon, Francois-Xavier; Braud, Emmanuelle; Fabis, Frederic; Lancelot, Jean-Charles; Rault, Sylvain
CORPORATE SOURCE: Centre d'Etudes et de Recherche sur le Medicament de Normandie, Caen, 14032, Fr.
SOURCE: Journal of Combinatorial Chemistry (2005), 7(2), 253-257
CODEN: JCCHFF; ISSN: 1520-4766
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



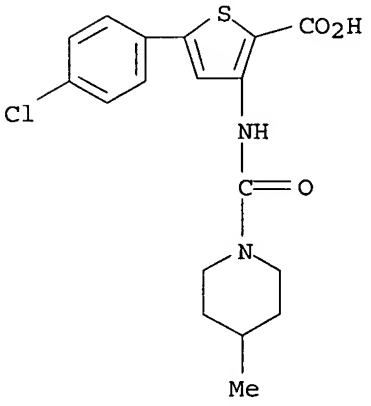
I

AB A 1140-library of thiophene ureido acids, e.g., I, was synthesized by the reaction of a set of 60 primary or secondary amines with a number of 19 thieno[3,2-d]- or thieno[2,3-d][1,3]oxazine-2,4-diones. All compds. were obtained by a simple solution-phase combinatorial strategy on a 200-400-mg scale with over 70% yields and purities over 80%. Sixty library members chosen at random were successfully characterized by standard 1H NMR, HPLC/MS, and IR studies. Analgesic, antalgic, and antiinflammatory potential were investigated. The 1140-member ureidothiophene carboxylic acid library will be used in high-throughput screening assays.

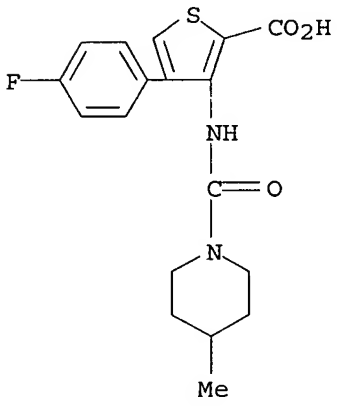
IT **649757-67-5P 845864-10-0P 845864-20-2P 845864-30-4P 845864-40-6P 845864-50-8P**

845864-60-0P 845864-70-2P 845864-80-4P
845865-39-6P 845865-45-4P 845865-93-2P
RL: CPN (Combinatorial preparation); CMBI (Combinatorial study); PREP (Preparation)
(solution-phase combinatorial preparation of ureidothiophenecarboxylic acids via nucleophilic ring opening of thiaisatoic anhydrides with amines)

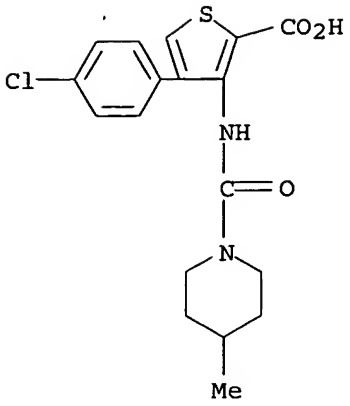
RN 649757-67-5 CAPLUS
CN 2-Thiophenecarboxylic acid, 5-(4-chlorophenyl)-3-[[(4-methyl-1-piperidinyl)carbonyl]amino]- (9CI) (CA INDEX NAME)



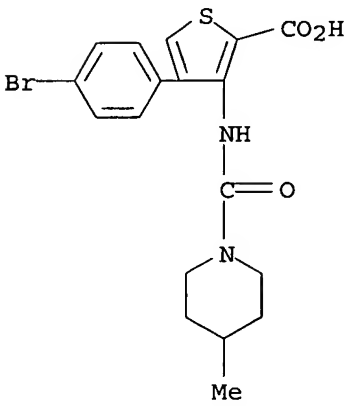
RN 845864-10-0 CAPLUS
CN 2-Thiophenecarboxylic acid, 4-(4-fluorophenyl)-3-[[(4-methyl-1-piperidinyl)carbonyl]amino]- (9CI) (CA INDEX NAME)



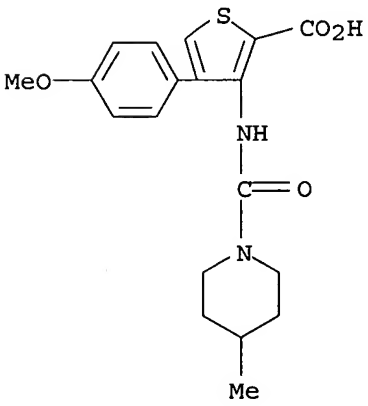
RN 845864-20-2 CAPLUS
CN 2-Thiophenecarboxylic acid, 4-(4-chlorophenyl)-3-[[(4-methyl-1-piperidinyl)carbonyl]amino]- (9CI) (CA INDEX NAME)



RN 845864-30-4 CAPLUS
CN 2-Thiophenecarboxylic acid, 4-(4-bromophenyl)-3-[[(4-methyl-1-piperidinyl)carbonyl]amino]- (9CI) (CA INDEX NAME)

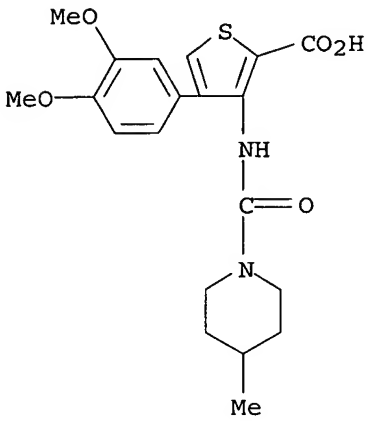


RN 845864-40-6 CAPLUS
CN 2-Thiophenecarboxylic acid, 4-(4-methoxyphenyl)-3-[[(4-methyl-1-piperidinyl)carbonyl]amino]- (9CI) (CA INDEX NAME)

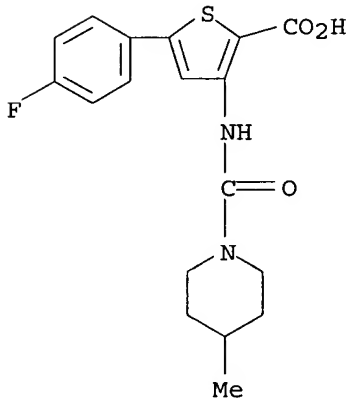


RN 845864-50-8 CAPLUS

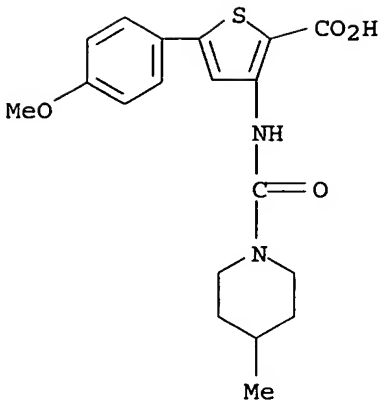
CN 2-Thiophenecarboxylic acid, 4-(3,4-dimethoxyphenyl)-3-[[(4-methyl-1-piperidinyl)carbonyl]amino]- (9CI) (CA INDEX NAME)



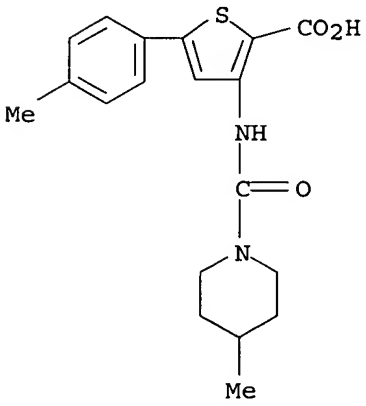
RN 845864-60-0 CAPLUS
CN 2-Thiophenecarboxylic acid, 5-(4-fluorophenyl)-3-[[(4-methyl-1-piperidinyl)carbonyl]amino]- (9CI) (CA INDEX NAME)



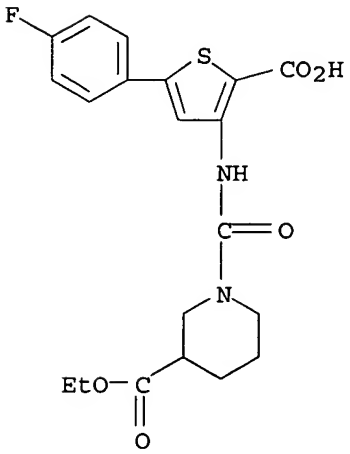
RN 845864-70-2 CAPLUS
CN 2-Thiophenecarboxylic acid, 5-(4-methoxyphenyl)-3-[[(4-methyl-1-piperidinyl)carbonyl]amino]- (9CI) (CA INDEX NAME)



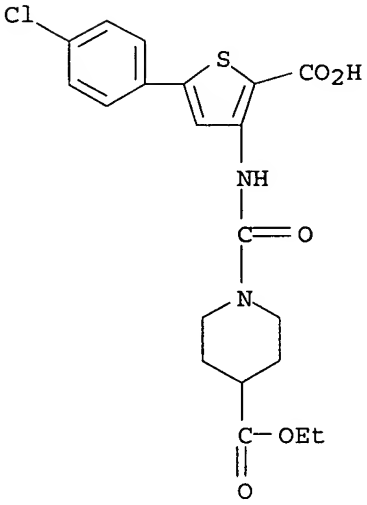
RN 845864-80-4 CAPLUS
CN 2-Thiophenecarboxylic acid, 5-(4-methylphenyl)-3-[[(4-methyl-1-piperidinyl)carbonyl]amino]- (9CI) (CA INDEX NAME)



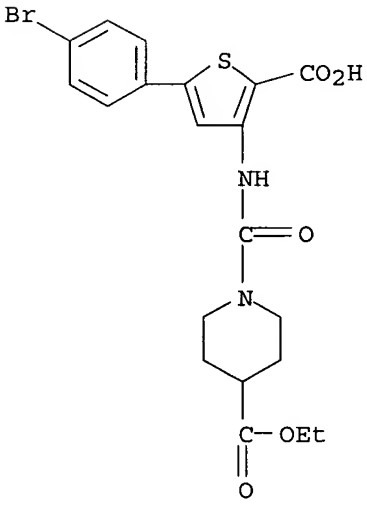
RN 845865-39-6 CAPLUS
CN 3-Piperidinecarboxylic acid, 1-[[[2-carboxy-5-(4-fluorophenyl)-3-thienyl]amino]carbonyl]-, 3-ethyl ester (9CI) (CA INDEX NAME)



RN 845865-45-4 CAPLUS
CN 4-Piperidinecarboxylic acid, 1-[[[2-carboxy-5-(4-chlorophenyl)-3-thienyl]amino]carbonyl]-, 4-ethyl ester (9CI) (CA INDEX NAME)



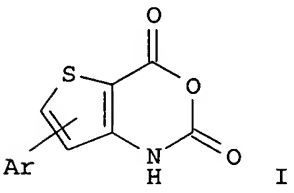
RN 845865-93-2 CAPLUS
CN 4-Piperidinecarboxylic acid, 1-[[[5-(4-bromophenyl)-2-carboxy-3-thienyl]amino]carbonyl]-, 4-ethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 4 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:900409 CAPLUS
DOCUMENT NUMBER: 140:128352
TITLE: Synthesis and combinatorial approach of the reactivity of 6- and 7-arylthieno[3,2-d][1,3]oxazine-2,4-diones
AUTHOR(S): Le Foulon, Francois-Xavier; Braud, Emmanuelle; Fabis,

Frederic; Lancelot, Jean-Charles; Rault, Sylvain
CORPORATE SOURCE: Centre d'Etudes et de Recherche sur le Medicament de Normandie 5, Caen, 14032, Fr.
SOURCE: Tetrahedron (2003), 59(50), 10051-10057
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:128352
GI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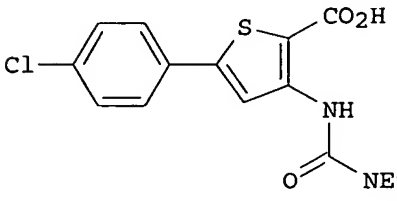
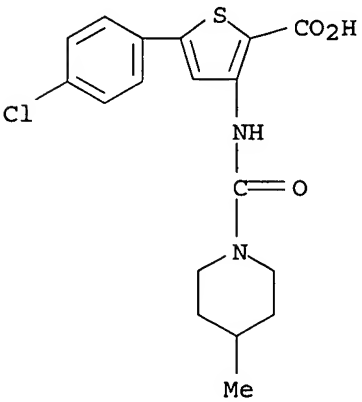

II

AB This paper describes a general procedure for the synthesis of new substituted thiaisatoic anhydrides or 6- or 7-aryl-1H-thieno[3,2-d][1,3]oxazine-2,4-diones I (Ar = Ph, 4-ClPh, 4-MePh, 2-thienyl, etc.). They were synthesized in large scale under microwave heating conditions with high yields. The reactivity vs nucleophilic reagents of these compds. was studied and permitted to develop a simple combinatorial procedure to synthesize a library of new thiophene ureidoacids, e.g., II.

IT **649757-67-5P**
RL: CPN (Combinatorial preparation); CMBI (Combinatorial study); PREP (Preparation)
(preparation of a combinatorial demonstration library of arylureidothiophencarboxylic acids via nucleophilic substitution of arylthieno-oxazinediones with amines)

RN 649757-67-5 CAPLUS
CN 2-Thiophenecarboxylic acid, 5-(4-chlorophenyl)-3-[[(4-methyl-1-piperidinyl)carbonyl]amino]- (9CI) (CA INDEX NAME)



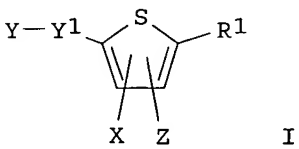
REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 5 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:964347 CAPLUS
DOCUMENT NUMBER: 138:24638
TITLE: Preparation of thiophenecarboxylic acids and methods for the treatment or prevention of flaviviridae infections such as hepatitis C
INVENTOR(S): Chan, Chun Kong Laval; Bedard, Jean; Das, Sanjoy Kumar; Nguyen Ba, Nghe; Pereira, Oswy Z.; Reddy, Thumkunta Jagadeeswar; Siddiqui, M. Arshad; Wang, Wuyi; Yannopoulos, Constantin
PATENT ASSIGNEE(S): Shire Biochem Inc., Can.
SOURCE: PCT Int. Appl., 314 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2002100851	A2	20021219	WO 2002-CA876		20020611
WO 2002100851	A3	20030227			
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM					
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
CA 2450007	AA	20021219	CA 2002-2450007		20020611
EP 1401825	A2	20040331	EP 2002-742563		20020611
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR					
US 2004116509	A1	20040617	US 2002-166031		20020611
US 6881741	B2	20050419			
BR 2002010357	A	20040629	BR 2002-10357		20020611
JP 2005500288	T2	20050106	JP 2003-503618		20020611
ZA 2003009590	A	20040512	ZA 2003-9590		20031210
PRIORITY APPLN. INFO.:			US 2001-296731P	P	20010611
			WO 2002-CA876	W	20020611

OTHER SOURCE(S): MARPAT 138:24638
GI



I

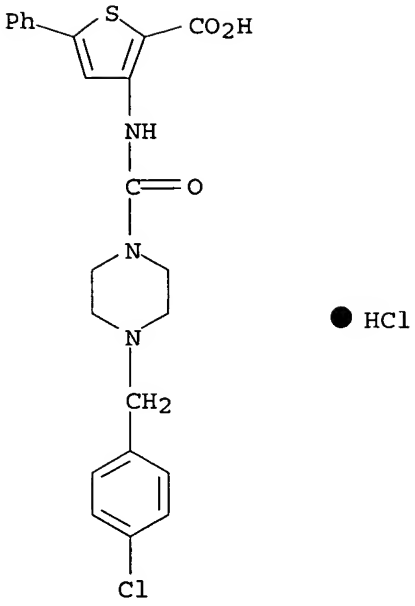
AB The present invention provides novel thiophenes (shown as I; variables defined below; e.g. 3-[(2-chlorophenylsulfonyl)amino]-5-phenylthiophene-2-carboxylic acid) or pharmaceutically acceptable salts thereof useful for treating flaviviridae viral infection. For I: X = -NR3MR2, -JNR2R3; M = -SO2-, -S(O)-, -S-, -C(O)-, -C(S)-, -C(O)NR4-, -C(S)NR15-, -CHR15-, -C(:NR8)-, a bond; R4 is C1-6 alkyl; R8 = H, C1-12 alkyl, C2-12 alkenyl,

C2-12 alkynyl, C6-14 aryl, C3-12 heterocycle, C3-12 heteroaralkyl, C6-16 aralkyl; and R15 = H or C1-6 alkyl; J = -C(:W)-, -CHR6-, -S-, -S(O)-, -SO2-; W = O, S or NR7, wherein R7 = H, C1-12 alkyl, C2-12 alkenyl, C2-12 alkynyl, C6-14 aryl, C3-12 heterocycle, C3-12 heteroaralkyl, C6-16 aralkyl; and R6 = H, C1-12 alkyl, C6-14 aryl or C6-16 aralkyl. Y1 = a bond, C1-6 alkyl, C2-6 alkenyl or C2-6 alkynyl; Y = COOR16, COCOOR5, P(O)ORaORb, S(O)OR5, S(O)2OR5, tetrazole, CON(R9)CH(R5)COOR5, CONR10R11, CON(R9)SO2R5, CONR9OH or halogen, wherein R9, R5, R10 and R11 = H, C1-12 alkyl, C2-12 alkenyl, C2-12 alkynyl, C3-12 heterocycle, C3-18 heteroaralkyl, C6-18 aralkyl; or R10 and R11 are taken together with the N to form a 3-10 membered heterocycle; Ra and Rb = H, C1-12 alkyl, C2-12 alkenyl, C2-12 alkynyl, C6-14 aryl, C3-12 heterocycle, C3-18 heteroaralkyl and C6-18 aralkyl; or Ra and Rb are taken together with the oxygens to form a 5-10 membered heterocycle. R16 = H, C1-12 alkyl, C2-12 alkenyl, C2-12 alkynyl, C6-14 aryl, C3-12 heterocycle, C3-18 heteroaralkyl and C6-18 aralkyl; provided that R16 is other than Me or Et; R1 = C2-12 alkyl, C2-12 alkenyl, C2-12 alkynyl, C6-14 aryl, C3-12 heterocycle, C3-18 heteroaralkyl or C6-18 aralkyl; R2 = C2-12 alkyl, C2-12 alkynyl, C6-14 aryl, C3-12 heterocycle, C3-18 heteroaralkyl, or C6-18 aralkyl; R3 = H, C1-12 alkyl, C2-12 alkenyl, C2-12 alkynyl, C6-14 aryl, C3-12 heterocycle, C3-18 heteroaralkyl or C6-18 aralkyl; Z = H, halogen, C1-6 alkyl; with provisos. Twenty-five example prepns. of I are included. For example, 3-[(2-chlorophenylsulfonyl)amino]-5-phenylthiophene-2-carboxylic acid was prepared by adding 1 N aqueous solution of LiOH.H2O (64.378 mmol) to a suspension of 3-amino-5-phenylthiophene-2-carboxylic acid Me ester (21.459 mmol) in a mixture of THF:MeOH:H2O (3:2:1, 75 mL) and stirring at 85° (external temperature) for 4 h. Solvents were removed under reduced pressure and the residue was partitioned between H2O and EtOAc. The H2O layer was separated and acidified with 1 N HCl solution and then EtOAc was added to it. The formed intermediate 3-amino-5-phenylthiophene-2-carboxylic acid (4.15 g, 88%; 0.457 mmol) was taken in a mixture of dioxane and H2O (1:1, 25 mL) and then Na carbonate (2.285 mmol) and 1-chlorophenylsulfonyl chloride (1.369 mmol) were added. The reaction mixture was stirred at room temperature for 12 h and eventually 69% of 3-[(2-chlorophenylsulfonyl)amino]-5-phenylthiophene-2-carboxylic acid was obtained. Results of evaluation of .apprx.580 I in the hepatitis C virus (HCV) RNA-dependent RNA polymerase and/or anti-helicase assays are tabulated.

IT **478023-94-8P**, 3-[[4-(4-Chlorobenzyl)piperazine-1-carbonyl]amino]-5-phenylthiophene-2-carboxylic acid monohydrochloride
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of thiophenecarboxylic acids and methods for treatment or prevention of flaviviridae infections such as hepatitis C)

RN 478023-94-8 CAPLUS

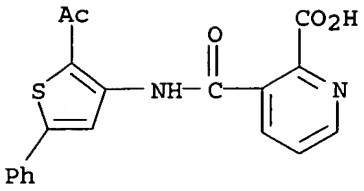
CN 2-Thiophenecarboxylic acid, 3-[[[4-[(4-chlorophenyl)methyl]-1-piperazinyl]carbonyl]amino]-5-phenyl-, monohydrochloride (9CI) (CA INDEX NAME)



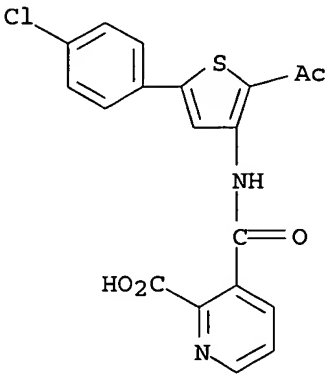
L18 ANSWER 6 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:646440 CAPLUS
DOCUMENT NUMBER: 138:153417
TITLE: Condensation products of 3-aminothiophenes with acid anhydrides
AUTHOR(S): Alkhathlan, Hamad Z.
CORPORATE SOURCE: Department of Chemistry, King Saud University, Riyadh, 11451, Saudi Arabia
SOURCE: Asian Journal of Chemistry (2002), 14(3-4), 1427-1435
CODEN: AJCHEW; ISSN: 0970-7077
PUBLISHER: Asian Journal of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:153417

AB Condensation of substituted 3-aminothiophenes with six different carboxylic acid anhydrides resulted in the formation of three types of products: N-(substituted thienyl) imides, substituted carboxylic acids and fused thieno[3,2-b]pyridines. Anhydrides included 5-nitro-1,3-isobenzofurandione, tetrachlorophthalic anhydride, 4,5,6,7-tetrahydro-1,3-isobenzofurandione, (3aR,7aS)-rel-3a,4,7,7a-tetrahydro-1,3-Isobenzofurandione and furo[3,4-c]pyridine-1,3-dione. Aminothiophene derivs. included 1-(3-amino-2-thienyl)ethanone, 1-(3-amino-5-phenyl-2-thienyl)ethanone, 1-[3-amino-5-(4-chlorophenyl)-2-thienyl]ethanone, and 1-[3-amino-5-(1,1-dimethylethyl)-2-thienyl]ethanone. The IR, NMR and MS spectra of these compds. are discussed.

IT **494864-62-9P 494864-63-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of condensation products of 1-(3-amino-2-thienyl)ethanone derivs. with anhydrides)
RN 494864-62-9 CAPLUS
CN 2-Pyridinecarboxylic acid, 3-[[(2-acetyl-5-phenyl-3-thienyl)amino]carbonyl]- (9CI) (CA INDEX NAME)



RN 494864-63-0 CAPLUS
CN 2-Pyridinecarboxylic acid, 3-[[[2-acetyl-5-(4-chlorophenyl)-3-thienyl]amino]carbonyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

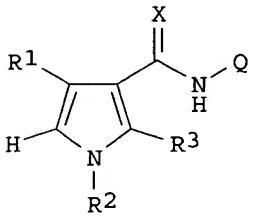
L18 ANSWER 7 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:368451 CAPLUS
DOCUMENT NUMBER: 136:369602
TITLE: Preparation of pyrrolecarboxamides and pyrrolecarbothioamides as agrochemical fungicides
INVENTOR(S): Walter, Harald
PATENT ASSIGNEE(S): Syngenta Participations A.-G., Switz.
SOURCE: PCT Int. Appl., 66 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002038542	A1	20020516	WO 2001-EP12830	20011106
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2426033	AA	20020516	CA 2001-2426033	20011106
AU 2002023668	A5	20020521	AU 2002-23668	20011106

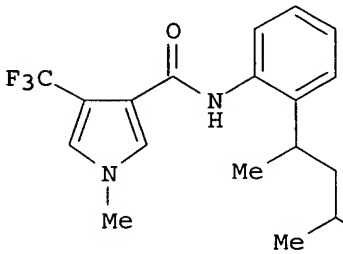
EP 1341757	A1	20030910	EP 2001-993599		20011106
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR					
BR 2001015200	A	20040217	BR 2001-15200		20011106
EG 23122	A	20040428	EG 2001-1173		20011106
JP 2004513163	T2	20040430	JP 2002-541078		20011106
US 2005119130	A1	20050602	US 2003-416219		20011106
ZA 2003003012	A	20040520	ZA 2003-3012		20030416
PRIORITY APPLN. INFO.:			GB 2000-27284	A	20001108
			GB 2000-30268	A	20001212
			WO 2001-EP12830	W	20011106

OTHER SOURCE(S): MARPAT 136:369602

GI



I



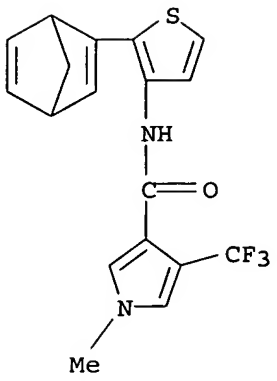
II

AB The title compds. [I; X = O, S; R1 = CF3, CF2H, CFH2; R2 = alkyl, haloalkyl, alkoxyalkyl, haloalkoxyalkyl; R3 = H, Me, CF3, F; Q = substituted Ph, 2-thienyl, 3-thienyl] which have plant-protecting properties and are suitable for protecting plants against infestation by phytopathogenic microorganisms, were prepared Thus, treating 1-methyl-4-trifluoromethylpyrrole-3-carboxylic acid with oxalyl chloride in the presence of a catalytic amount of DMF in CH2Cl2 followed by addition of the resulting acid chloride to a solution of 2-(1,3-dimethylbutyl)phenylamine and Et3N in CH2Cl2 afforded II. Compds. I showed good activity (< 20% infestation) against Puccinia recondita (brown rust) on wheat.

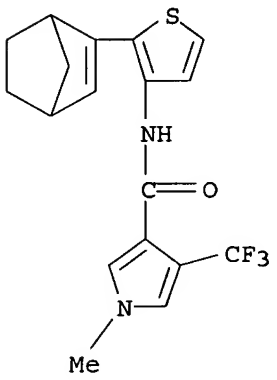
IT **424832-60-0P 424832-61-1P 424832-62-2P**
424832-63-3P 424832-64-4P 424832-65-5P
424832-66-6P 424832-67-7P 424832-68-8P
424832-69-9P 424832-70-2P 424832-71-3P
424832-72-4P 424832-73-5P 424832-74-6P
424832-75-7P 424832-76-8P 424832-77-9P
424832-78-0P 424832-79-1P 424832-80-4P
424832-81-5P 424832-82-6P 424832-83-7P
424832-84-8P
RL: AGR (Agricultural use); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrrolecarboxamides and pyrrolecarbothioamides as agrochem. fungicides)

RN 424832-60-0 CAPLUS

CN 1H-Pyrrole-3-carboxamide, N-(2-bicyclo[2.2.1]hepta-2,5-dien-2-yl-3-thienyl)-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

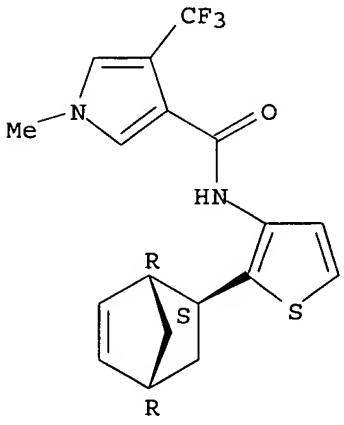


RN 424832-61-1 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-(2-bicyclo[2.2.1]hept-2-en-2-yl-3-thienyl)-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 424832-62-2 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[2-(1R,2S,4R)-bicyclo[2.2.1]hept-5-en-2-yl-3-thienyl]-1-methyl-4-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

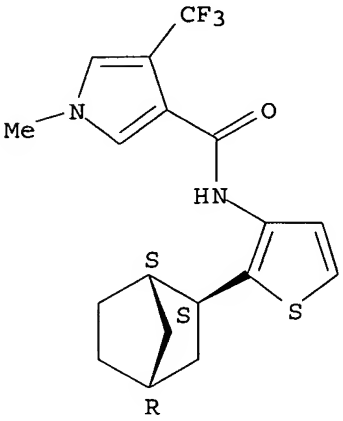
Relative stereochemistry.



RN 424832-63-3 CAPLUS

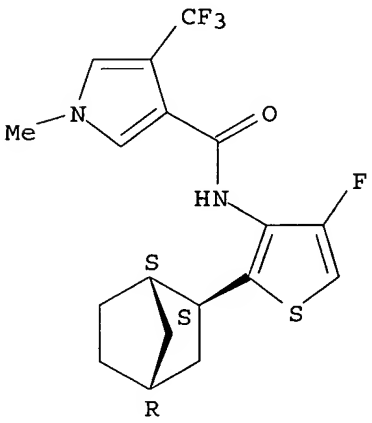
CN 1H-Pyrrole-3-carboxamide, N-[2-(1R,2R,4S)-bicyclo[2.2.1]hept-2-yl-3-thienyl]-1-methyl-4-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



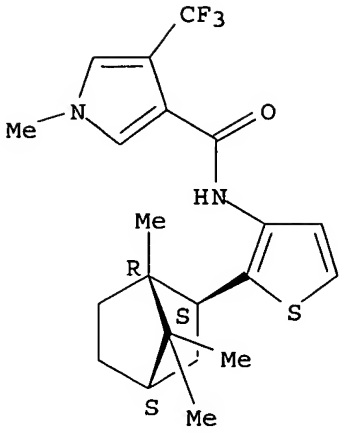
RN 424832-64-4 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[2-(1R,2R,4S)-bicyclo[2.2.1]hept-2-yl-4-fluoro-3-thienyl]-1-methyl-4-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



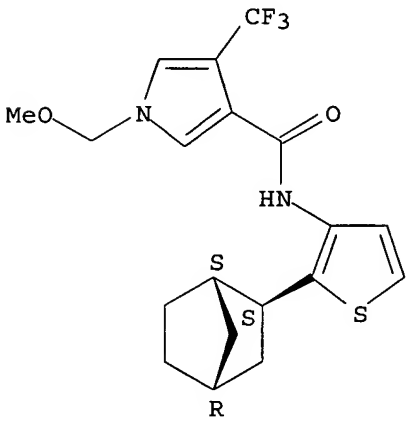
RN 424832-65-5 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 1-methyl-4-(trifluoromethyl)-N-[2-[(1R,2S,4S)-1,7,7-trimethylbicyclo[2.2.1]hept-2-yl]-3-thienyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



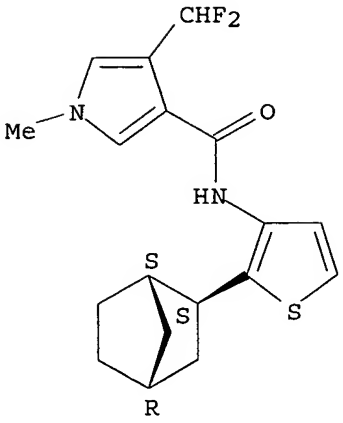
RN 424832-66-6 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[2-(1R,2R,4S)-bicyclo[2.2.1]hept-2-yl-3-thienyl]-1-(methoxymethyl)-4-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

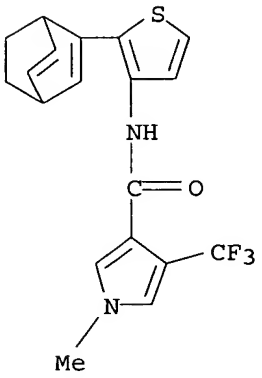


RN 424832-67-7 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[2-(1R,2R,4S)-bicyclo[2.2.1]hept-2-yl-3-thienyl]-4-(difluoromethyl)-1-methyl-, rel- (9CI) (CA INDEX NAME)

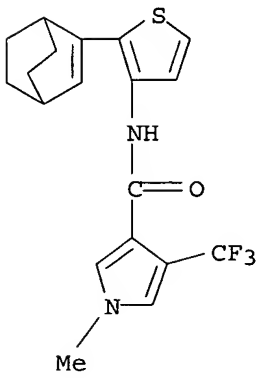
Relative stereochemistry.



RN 424832-68-8 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-(2-bicyclo[2.2.2]octa-2,5-dien-2-yl-3-thienyl)-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)



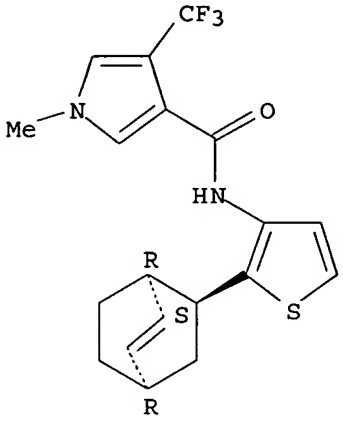
RN 424832-69-9 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-(2-bicyclo[2.2.2]oct-2-en-2-yl-3-thienyl)-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)



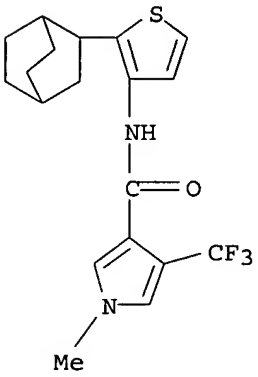
RN 424832-70-2 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[2-(1R,2S,4R)-bicyclo[2.2.2]oct-5-en-2-yl-3-

thienyl]-1-methyl-4-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

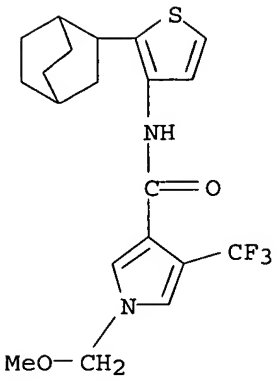
Relative stereochemistry.



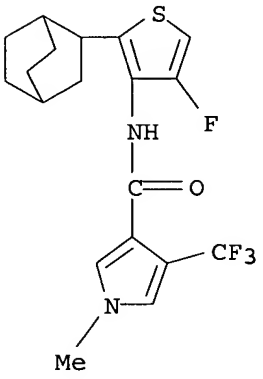
RN 424832-71-3 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-(2-bicyclo[2.2.2]oct-2-yl-3-thienyl)-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)



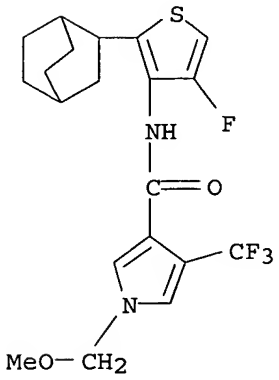
RN 424832-72-4 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-(2-bicyclo[2.2.2]oct-2-yl-3-thienyl)-1-(methoxymethyl)-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 424832-73-5 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-(2-bicyclo[2.2.2]oct-2-yl-4-fluoro-3-thienyl)-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

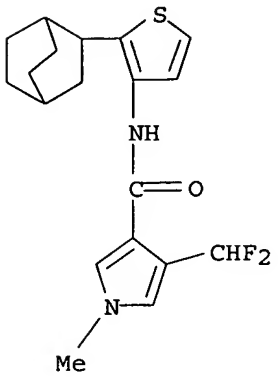


RN 424832-74-6 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-(2-bicyclo[2.2.2]oct-2-yl-4-fluoro-3-thienyl)-1-(methoxymethyl)-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)



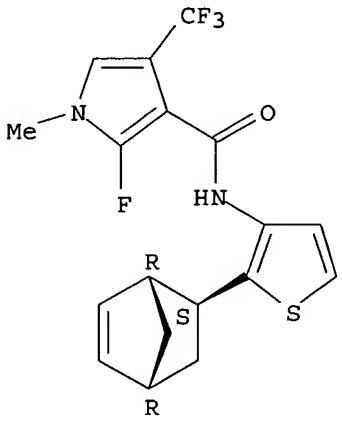
RN 424832-75-7 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-(2-bicyclo[2.2.2]oct-2-yl-3-thienyl)-4-

(difluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)



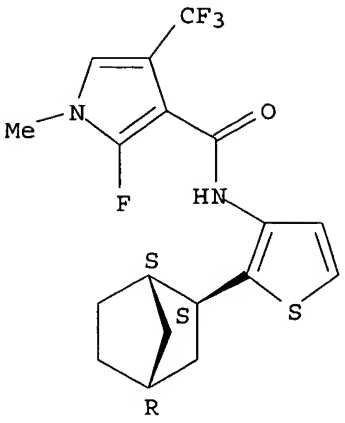
RN 424832-76-8 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[2-(1R,2S,4R)-bicyclo[2.2.1]hept-5-en-2-yl-3-thienyl]-2-fluoro-1-methyl-4-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



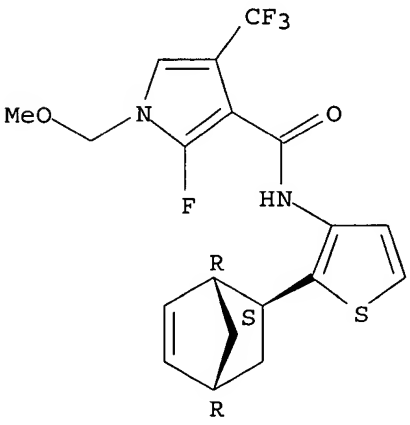
RN 424832-77-9 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[2-(1R,2R,4S)-bicyclo[2.2.1]hept-2-yl-3-thienyl]-2-fluoro-1-methyl-4-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



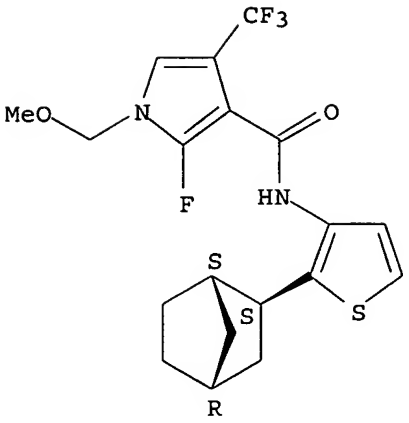
RN 424832-78-0 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[2-(1R,2S,4R)-bicyclo[2.2.1]hept-5-en-2-yl-3-thienyl]-2-fluoro-1-(methoxymethyl)-4-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



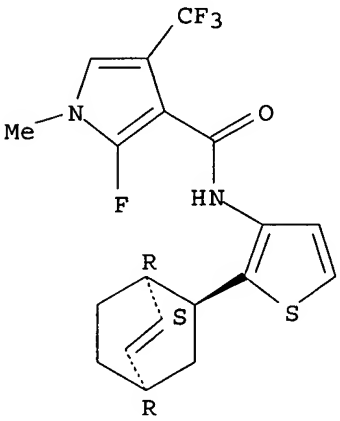
RN 424832-79-1 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[2-(1R,2R,4S)-bicyclo[2.2.1]hept-2-yl-3-thienyl]-2-fluoro-1-(methoxymethyl)-4-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

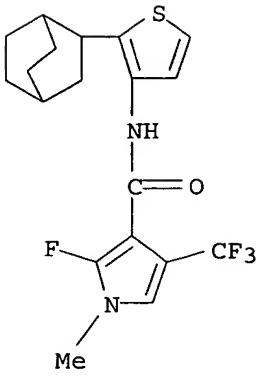


RN 424832-80-4 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[2-(1R,2S,4R)-bicyclo[2.2.2]oct-5-en-2-yl-3-thienyl]-2-fluoro-1-methyl-4-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

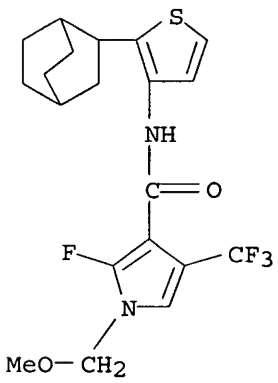
Relative stereochemistry.



RN 424832-81-5 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-(2-bicyclo[2.2.2]oct-2-yl-3-thienyl)-2-fluoro-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

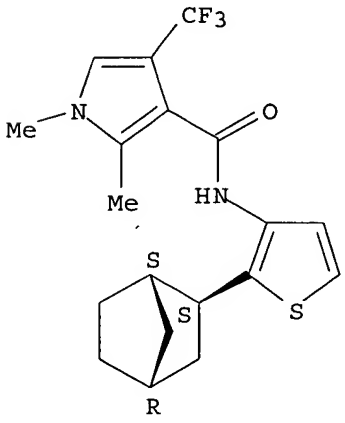


RN 424832-82-6 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-(2-bicyclo[2.2.2]oct-2-yl-3-thienyl)-2-fluoro-1-(methoxymethyl)-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

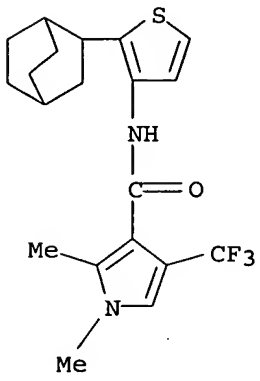


RN 424832-83-7 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[2-(1R,2R,4S)-bicyclo[2.2.1]hept-2-yl-3-thienyl]-1,2-dimethyl-4-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 424832-84-8 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-(2-bicyclo[2.2.2]oct-2-yl-3-thienyl)-1,2-dimethyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)



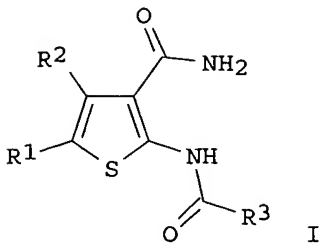
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 8 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:935593 CAPLUS
DOCUMENT NUMBER: 136:69729
TITLE: Preparation of thiophene-3-carboxamides as kinase inhibitors
INVENTOR(S): Fancelli, Daniele; Pevarello, Paolo; Varasi, Mario
PATENT ASSIGNEE(S): Pharmacia & Upjohn S.p.A., Italy
SOURCE: PCT Int. Appl., 85 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001098290	A2	20011227	WO 2001-EP6763	20010614
WO 2001098290	A3	20020516		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6414013	B1	20020702	US 2000-596550	20000619
CA 2414085	AA	20011227	CA 2001-2414085	20010614
AU 2001085745	A5	20020102	AU 2001-85745	20010614
EP 1294707	A2	20030326	EP 2001-964983	20010614
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2004501146	T2	20040115	JP 2002-504246	20010614
PRIORITY APPLN. INFO.:			US 2000-596550 A	20000619
			WO 2001-EP6763 W	20010614

OTHER SOURCE(S): MARPAT 136:69729

GI



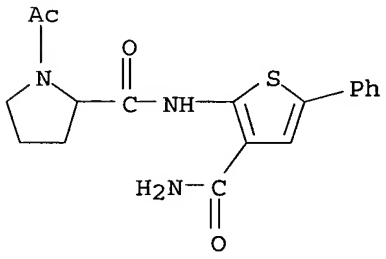
I

AB The title compds. [I; R1, R2 = H, halo, aryl, etc.; or R1 and R2 taken together form (CH2)m(NR4)n(CH2)p (wherein m, p = 1-3; n = 0-1; m + n + p = 3-5; R4 = H, alkyl); R3 = alkyl, alkenyl, aryl, etc.], useful in the treatment of diseases caused by and/or associated with an altered protein kinase activity such as cancer, cell proliferative disorders, Alzheimer's disease, viral infections, auto-immune diseases and neurodegenerative disorders (no data given), were prepared Thus, amidation of 2-amino-3-carbamoyl-4,5,6,7-tetrahydrobenzo[b]thiophene with phenylacetic acid afforded I [R1R2 = (CH2)4; R3 = CH2Ph].

IT **383380-21-0P 383380-23-2P 383380-24-3P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of thiophene-3-carboxamides as kinase inhibitors)

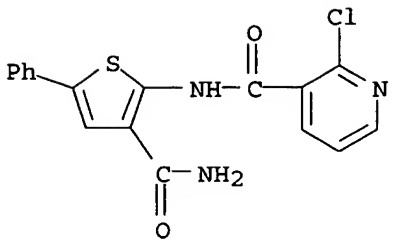
RN 383380-21-0 CAPLUS

CN 2-Pyrrolidinecarboxamide, 1-acetyl-N-[3-(aminocarbonyl)-5-phenyl-2-thienyl]- (9CI) (CA INDEX NAME)

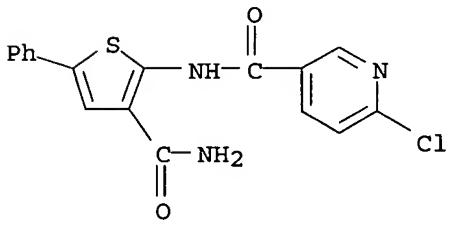


RN 383380-23-2 CAPLUS

CN 3-Pyridinecarboxamide, N-[3-(aminocarbonyl)-5-phenyl-2-thienyl]-2-chloro- (9CI) (CA INDEX NAME)



RN 383380-24-3 CAPLUS
CN 3-Pyridinecarboxamide, N-[3-(aminocarbonyl)-5-phenyl-2-thienyl]-6-chloro-
(9CI) (CA INDEX NAME)

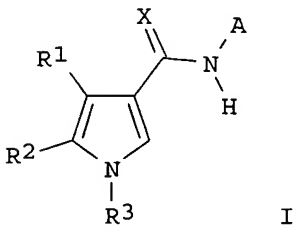


L18 ANSWER 9 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:545661 CAPLUS
DOCUMENT NUMBER: 135:137397
TITLE: Preparation of pyrrolecarboxamides and pyrrolethioamides as fungicides
INVENTOR(S): Walter, Harald; Schneider, Hermann
PATENT ASSIGNEE(S): Syngenta Participations A.-G., Switz.
SOURCE: PCT Int. Appl., 111 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001053259	A1	20010726	WO 2001-EP592	20010119
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2397008	AA	20010726	CA 2001-2397008	20010119
BR 2001007738	A	20021022	BR 2001-7738	20010119
EP 1252140	A1	20021030	EP 2001-907468	20010119
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003520269	T2	20030702	JP 2001-553263	20010119

AU 772635	B2	20040506	AU 2001-35433		20010119
ZA 2002005641	A	20031103	ZA 2002-5641		20020715
US 2004049035	A1	20040311	US 2002-181702		20021008
US 6806286	B2	20041019			
US 2004106521	A1	20040603	US 2003-680346		20031007
PRIORITY APPLN. INFO.:			GB 2000-1447	A	20000121
			WO 2001-EP592	W	20010119
			US 2002-181702	A3	20021008

OTHER SOURCE(S): MARPAT 135:137397
GI

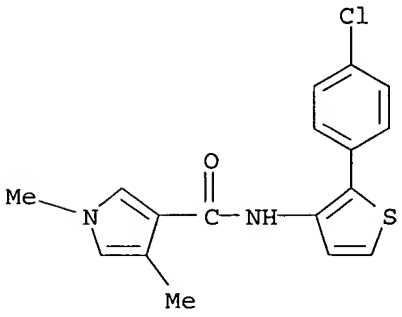


I

AB The title compds. [I; X = O, S; R1 = alkyl, cycloalkyl, halo; R2 = H, alkyl, alkoxy, etc.; R3 = alkyl; A = (un)substituted ortho-substituted (hetero)aryl, bicyclo(hetero)aryl] which have plant-protective properties and are suitable for protecting plants against infestations by phytopathogenic microorganisms, were prepared Thus, methylation of Me 4-methylpyrrole-3-carboxylate followed by hydrolysis of the resulting ester, and reaction of 1,4-dimethylpyrrole-3-carboxylic acid with 2-(4'-fluorophenyl)aniline afforded I [X = O; R1, R3 = Me; R2 = H; A = 4'-fluorobiphenyl-2-yl] which showed strong efficacy against Puccinia recondita on wheat (< 20% infestation).

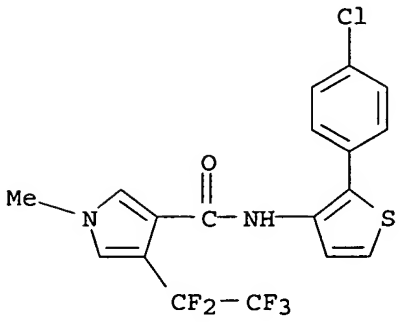
IT **351416-74-5P 351416-75-6P 351416-76-7P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrrolecarboxamides and pyrrolethioamides as fungicides)

RN 351416-74-5 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[2-(4-chlorophenyl)-3-thienyl]-1,4-dimethyl- (9CI) (CA INDEX NAME)

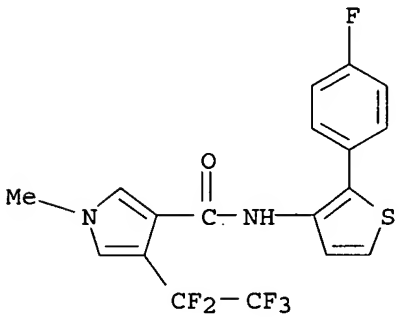


RN 351416-75-6 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[2-(4-chlorophenyl)-3-thienyl]-1-methyl-4-

(pentafluoroethyl)- (9CI) (CA INDEX NAME)



RN 351416-76-7 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[2-(4-fluorophenyl)-3-thienyl]-1-methyl-4-(pentafluoroethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 10 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:507677 CAPLUS
DOCUMENT NUMBER: 135:92539
TITLE: Preparation of trifluoromethylpyrrole carboxamides and trifluoromethylpyrrolethioamides as fungicides
INVENTOR(S): Walter, Harald; Trah, Stephan; Schneider, Hermann
PATENT ASSIGNEE(S): Syngenta Participations A.-G., Switz.
SOURCE: PCT Int. Appl., 65 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

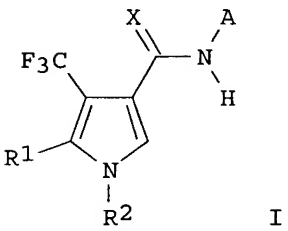
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001049664	A1	20010712	WO 2000-EP11196	20001111

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG						
CA 2395267		AA	20010712	CA 2000-2395267		20001111
BR 2000016871		A	20021008	BR 2000-16871		20001111
EP 1252139		A1	20021030	EP 2000-985016		20001111
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR						
JP 2003519212		T2	20030617	JP 2001-550204		20001111
EG 22599		A	20030430	EG 2000-1588		20001224
ZA 2002004874		A	20030918	ZA 2002-4874		20020618
US 6699818		B1	20040302	US 2002-169281		20021008
US 2004171490		A1	20040902	US 2004-785836		20040224
PRIORITY APPLN. INFO.:				GB 1999-30750	A	19991229
				WO 2000-EP11196	W	20001111
				US 2002-169281	A3	20021008

OTHER SOURCE(S): MARPAT 135:92539

GI



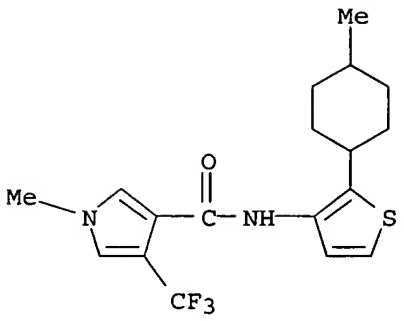
I

AB The title compds. [I; X = O, S; R1 = H, alkyl, halo; R2 = alkyl; A = ortho-substituted aryl, ortho-substituted heteroaryl, bicycloaryl, bicycloheteroaryl] which have plant-protective properties and are suitable for protecting plants against infestations by phytopathogenic microorganisms, were prepared E.g., a multi-step synthesis of I [R1 = H; R2 = Me; X = O; A = 4-(4-chlorophenyl)pyridin-3-yl] which showed strong efficacy against Erypsiphe graminis on barley, was given.

IT **349486-95-9P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of trifluoromethylpyrrole carboxamides and trifluoromethylpyrrolethioamides as fungicides)

RN 349486-95-9 CAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-methyl-N-[2-(4-methylcyclohexyl)-3-thienyl]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)



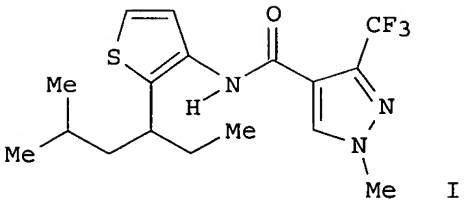
REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 11 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:665606 CAPLUS
DOCUMENT NUMBER: 133:237849
TITLE: Preparation of 3-acylamino-2-alkylthiophenes
INVENTOR(S): Katsuta, Hiroyuki; Ishii, Seiichi; Tomiya, Kanji; Kodaka, Kenji
PATENT ASSIGNEE(S): Mitsui Chemicals, Inc., Japan
SOURCE: Eur. Pat. Appl., 102 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1036793	A2	20000920	EP 2000-105331	20000316
EP 1036793	A3	20010228		
EP 1036793	B1	20050907		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2000327678	A2	20001128	JP 2000-55200	20000301
IN 187208	A	20020302	IN 2000-MU190	20000306
US 6239282	B1	20010529	US 2000-524007	20000313
CN 1267671	A	20000927	CN 2000-104097	20000316
BR 2000001744	A	20001031	BR 2000-1744	20000316
CN 1495180	A	20040512	CN 2003-124126	20000316
EP 1559714	A1	20050803	EP 2004-11763	20000316
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY				
AT 304004	E	20050915	AT 2000-105331	20000316
US 6331634	B1	20011218	US 2000-694837	20001024
US 2001023295	A1	20010920	US 2001-785320	20010220
US 6331639	B2	20011218		
IN 190496	A	20030802	IN 2001-MU554	20010618
IN 190570	A	20030809	IN 2001-MU555	20010618

PRIORITY APPLN. INFO.:
JP 1999-69387 A 19990316
IN 2000-MU190 A 20000306
US 2000-524007 A3 20000313
EP 2000-105331 A3 20000316

OTHER SOURCE(S): CASREACT 133:237849; MARPAT 133:237849
GI



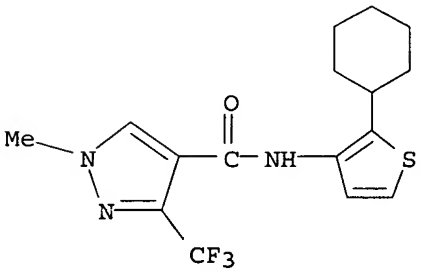
I

AB R1CHR2CH(CHR3R4)ZNHCOR [R = H, alkyl, alkoxy, (hetero)aryl, etc.; R1-R4 = H or alkyl; R1R2,R1R3, R2R3, etc. = alkylene; Z = thiophene-2,3-diyl] were prepared by condensation of HZNHCOR with R1CHR2COCHR3R4 followed by hydrogenation. Thus, Me 3-aminothiophene-2-carboxylate was N-acylated by 3-trifluoromethyl-1-methylpyrazole-4-carbonyl chloride and the saponified product decarboxylated to give N-(3-thienyl)-3-trifluoromethyl-1-methylpyrazole-4-carboxamide which was condensed with Me2CHCH2COMe and the product mixture hydrogenated to give title compd I.

IT **239093-65-3P**
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of 3-acylamino-2-alkylthiophenes)

RN 239093-65-3 CAPLUS

CN 1H-Pyrazole-4-carboxamide, N-(2-cyclohexyl-3-thienyl)-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



L18 ANSWER 12 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:241135 CAPLUS

DOCUMENT NUMBER: 132:279106

TITLE: Non-peptide GnRH agents, methods and intermediates for their preparation

INVENTOR(S): Anderson, Mark Brian; Vazir, Haresh N.; Luthin, David Robert; Paderes, Genevieve Deguzman; Pathak, Ved P.; Christie, Lance Christopher; Hong, Yufeng; Tompkins, Eileen Valenzuela; Li, Haitao; Faust, James

PATENT ASSIGNEE(S): Agouron Pharmaceuticals, Inc., USA; et al.

SOURCE: PCT Int. Appl., 444 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

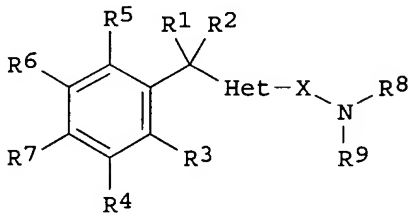
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

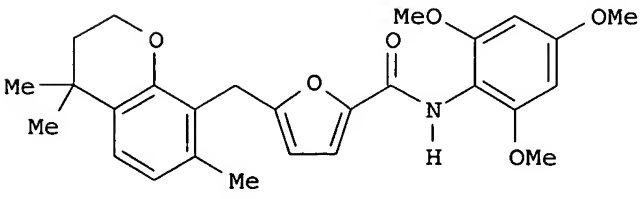
WO 2000020358	A2	20000413	WO 1999-US18790		19990820
WO 2000020358	A3	20001116			
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM					
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG					
CA 2341346	AA	20000413	CA 1999-2341346		19990820
BR 9913374	A	20010515	BR 1999-13374		19990820
EP 1105120	A2	20010613	EP 1999-968010		19990820
EP 1105120	B1	20050323			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO					
EE 200100102	A	20020617	EE 2001-102		19990820
SI 20746	C	20020630	SI 1999-20076		19990820
TR 200100631	T2	20020821	TR 2001-200100631		19990820
JP 2002535244	T2	20021022	JP 2000-574479		19990820
AU 759310	B2	20030410	AU 2000-24709		19990820
NZ 509252	A	20040528	NZ 1999-509252		19990820
AT 291423	E	20050415	AT 1999-968010		19990820
ES 2237966	T3	20050801	ES 1999-968010		19990820
NO 2001000309	A	20010411	NO 2001-309		20010119
ZA 2001000831	A	20020822	ZA 2001-831		20010130
LV 12732	B	20020320	LV 2001-45		20010316
BG 105362	A	20011231	BG 2001-105362		20010319
LT 4904	B	20020425	LT 2001-24		20010319
US 2004010033	A1	20040115	US 2003-353160		20030708
PRIORITY APPLN. INFO.:			US 1998-97520P	P	19980820
			WO 1999-US18790	W	19990820
			US 2001-763216	B3	20010220

OTHER SOURCE(S): MARPAT 132:279106

GI



I



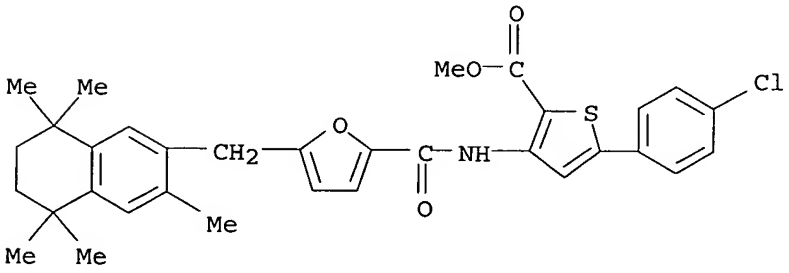
II

AB Non-peptide GnRH agents capable of inhibiting the effect of gonadotropin-releasing hormone are described. The compds. and their pharmaceutically acceptable salts, multimers, prodrugs, and active metabolites are suitable for treating mammalian reproductive disorders and steroid hormone-dependent tumors as well as for regulating fertility, where suppression of gonadotropin release is indicated. The compds. include those of formula I [X = C:O, C:S, S:O, or SO2; Het = 5-membered NOS-heterocycle; R1, R2 = H, alkyl; R3-R7 = H, halo, (un)substituted alkyl, aryl, heteroaryl, CH2OR, OR, CO2R; R = alkyl, aryl, etc.; adjacent rings positions such as R6R7 may form (un)substituted 5- or 6-membered ring with up to 4 heteroatoms; R8 = lipophilic moiety such as alkyl, aryl, CH2OR, OR, etc.; R9 = H, (un)substituted alkyl]. Methods and intermediates for synthesizing the compds. are also described. For instance, 4,4,7-trimethylchroman (preparation given) was alkylated in the 6- and 8-positions using Et 5-(chloromethyl)-2-furoate (46% total yield), and the resulting esters were hydrolyzed to a mixture of acids. This unsepd. mixture was treated with SOCl2 and amidated with 2,4,6-trimethoxyphenylamine-HCl to give the invention compound II and its chroman-6-position isomer, which were separated by HPLC. Several compds. exhibited high affinity (<100 nM) at human GnRH receptors. The compds. antagonized GnRH-stimulated inositol phosphate accumulation in cells with recombinant human GnRH receptors, and an example compound reduced plasma LH levels in castrated male rats. Various biol. data for several hundred compds. are given.

IT **263856-92-4P 263856-95-7P 263856-99-1P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(target compound; preparation of non-peptide GnRH agents for regulating gonadotropin secretion)

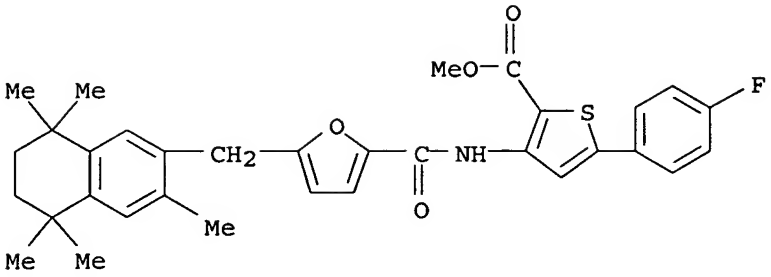
RN 263856-92-4 CAPLUS

CN 2-Thiophenecarboxylic acid, 5-(4-chlorophenyl)-3-[[[5-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)methyl]-2-furanyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

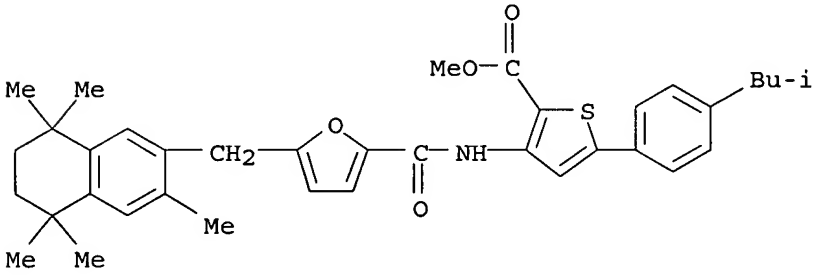


RN 263856-95-7 CAPLUS

CN 2-Thiophenecarboxylic acid, 5-(4-fluorophenyl)-3-[[[5-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)methyl]-2-furanyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 263856-99-1 CAPLUS
CN 2-Thiophenecarboxylic acid, 5-[4-(2-methylpropyl)phenyl]-3-[[[5-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)methyl]-2-furanyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



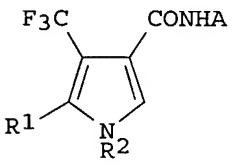
L18 ANSWER 13 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:133660 CAPLUS
DOCUMENT NUMBER: 132:166122
TITLE: (Trifluoromethyl)pyrrolecarboxamides
INVENTOR(S): Eberle, Martin; Walter, Harald
PATENT ASSIGNEE(S): Novartis A.-G., Switz.; Novartis-Erfindungen Verwaltungsgesellschaft m.b.H.
SOURCE: PCT Int. Appl., 35 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000009482	A1	20000224	WO 1999-EP5837	19990810
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
TW 576831	B	20040221	TW 1999-88107745	19990513
AU 9955138	A1	20000306	AU 1999-55138	19990810
AU 756140	B2	20030102		

BR 9912962	A	20010508	BR 1999-12962		19990810
EP 1105375	A1	20010613	EP 1999-941573		19990810
EP 1105375	B1	20060222			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY					
TR 200100478	T2	20010621	TR 2001-200100478		19990810
JP 2002522526	T2	20020723	JP 2000-564936		19990810
RU 2264388	C2	20051120	RU 2001-105955		19990810
US 2002019541	A1	20020214	US 2001-780897		20010209
US 6365620	B2	20020402			
PRIORITY APPLN. INFO.:			GB 1998-17548	A	19980812
			WO 1999-EP5837	W	19990810

OTHER SOURCE(S): MARPAT 132:166122

GI



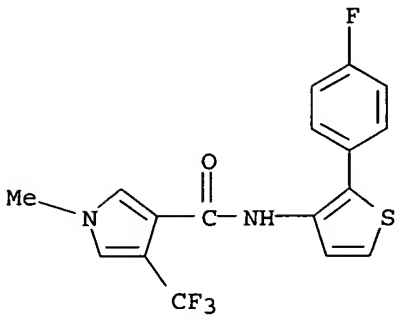
I

AB Title compds. I (R1 = H, halo, alkyl, haloalkyl; R2 = alkyl, haloalkyl, alkoxyalkyl, cyano, alkylsulfonyl, arylsulfonyl, etc.; A = substituted Ph, substituted 3-thienyl, substituted 4-indanyl) were prepared as plant protectants. Thus, 1.9 g 1-methyl-4-(trifluoromethyl)pyrrole-3-carboxylic acid, obtained from Et 4,4,4-trifluorocrotonate, tosylmethyl isocyanide, and MeI, and 0.9 mL oxalyl chloride in 20 mL CH2Cl2 was stirred at room temperature in the presence of a catalytic amount of DMF, the solvent was evaporated under reduced pressure to give a crystalline solid, and the solid was added to a solution of 1.7 g of 2-biphenylamine and 4.2 mL Et3N in 20 mL CH2Cl2 at 0°, and the reaction mixture was stirred for 2 h at room temperature to give I (R1 = H, R2 = Me, A = 2-biphenylyl). Application of this compound on apples, grapes, and tomatoes resulted in <10% infestation by Botrytis cinerea.

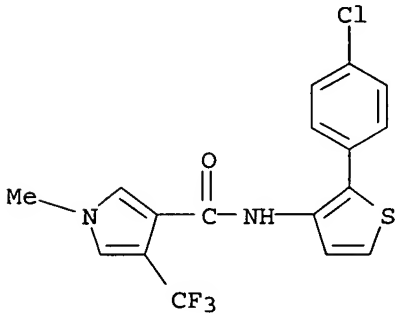
IT **258510-88-2P 258510-89-3P 258510-91-7P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
((trifluoromethyl)pyrrolecarboxamides as plant protectants)

RN 258510-88-2 CAPLUS

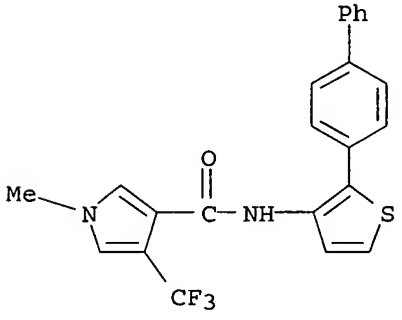
CN 1H-Pyrrole-3-carboxamide, N-[2-(4-fluorophenyl)-3-thienyl]-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 258510-89-3 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[2-(4-chlorophenyl)-3-thienyl]-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 258510-91-7 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-(2-[1,1'-biphenyl]-4-yl-3-thienyl)-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)



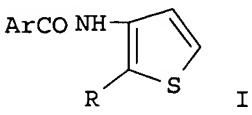
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 14 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:531012 CAPLUS
DOCUMENT NUMBER: 131:170262
TITLE: Preparation of thiophene derivatives as fungicides
INVENTOR(S): Yoshikawa, Yukihiro; Katsuta, Hiroyuki; Kitajima, Toshio; Tomitani, Kanji; Yanase, Yuji; Kawashima, Hideo

PATENT ASSIGNEE(S): Mitsui Chemicals Inc., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 12 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 11228567	A2	19990824	JP 1998-34925	19980217
PRIORITY APPLN. INFO.:			JP 1998-34925	19980217

OTHER SOURCE(S): MARPAT 131:170262
GI

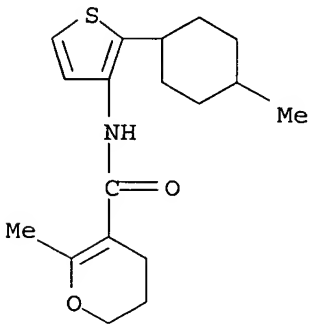


I

AB Thiophnes I [R = (un)substituted cycloalkyl; Ar = (un)substituted thiazolyl, pyrazolyl, furyl, etc.], useful as fungicides, were prepared Thus, reaction of 2-(3-methylcyclopentyl)-3-thienylamine with 3-trifluoromethyl-1-methylpyrazole-4-carboxylic acid chloride in pyridine at room temperature for 1 h gave N-[2-(3-methylcyclopentyl)-3-thienyl]-3-trifluoromethyl-1-methylpyrazole-4-carboxamide (II). II showed fungicidal activity against Puccinia recondita at 200 ppm.

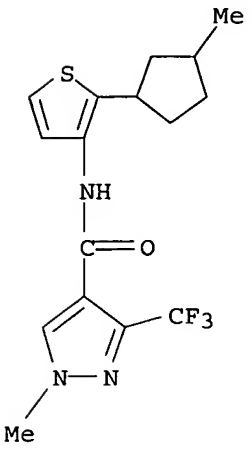
IT **239093-69-7**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study); USES (Uses)
(preparation of thiophene derivs. as fungicides)

RN 239093-69-7 CAPLUS
CN 2H-Pyran-5-carboxamide, 3,4-dihydro-6-methyl-N-[2-(4-methylcyclohexyl)-3-thienyl]- (9CI) (CA INDEX NAME)

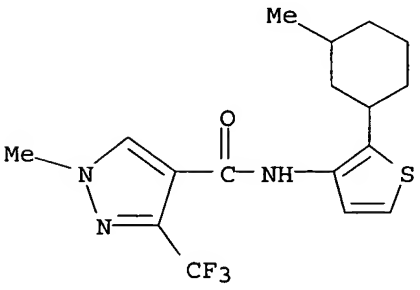


IT **239093-63-1P 239093-64-2P 239093-65-3P**
239093-66-4P 239093-67-5P 239093-68-6P
239093-70-0P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

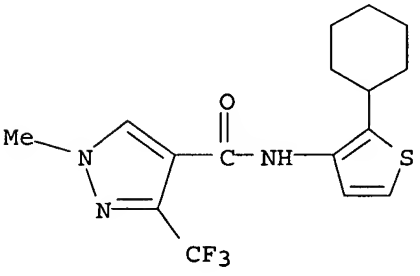
(preparation of thiophene derivs. as fungicides)
RN 239093-63-1 CAPLUS
CN 1H-Pyrazole-4-carboxamide, 1-methyl-N-[2-(3-methylcyclopentyl)-3-thienyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 239093-64-2 CAPLUS
CN 1H-Pyrazole-4-carboxamide, 1-methyl-N-[2-(3-methylcyclohexyl)-3-thienyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

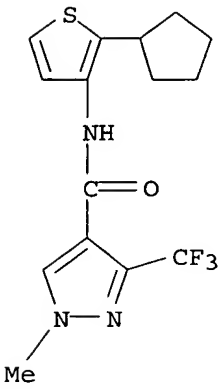


RN 239093-65-3 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-(2-cyclohexyl-3-thienyl)-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

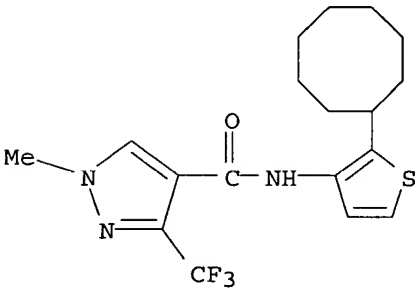


RN 239093-66-4 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-(2-cyclopentyl-3-thienyl)-1-methyl-3-

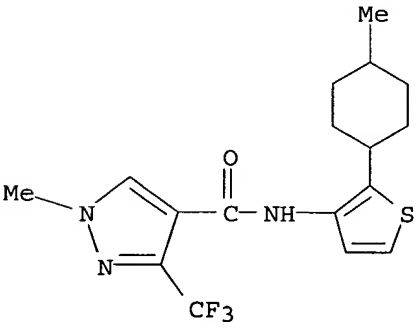
(trifluoromethyl)- (9CI) (CA INDEX NAME)



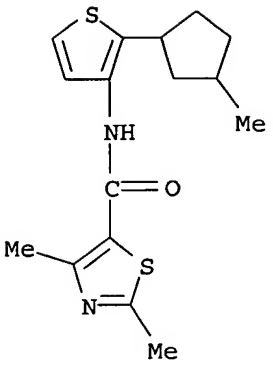
RN 239093-67-5 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-(2-cyclooctyl-3-thienyl)-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 239093-68-6 CAPLUS
CN 1H-Pyrazole-4-carboxamide, 1-methyl-N-[2-(4-methylcyclohexyl)-3-thienyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



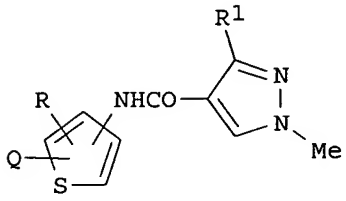
RN 239093-70-0 CAPLUS
CN 5-Thiazolecarboxamide, 2,4-dimethyl-N-[2-(3-methylcyclopentyl)-3-thienyl]- (9CI) (CA INDEX NAME)



L18 ANSWER 15 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:754357 CAPLUS
DOCUMENT NUMBER: 128:22908
TITLE: Preparation of N-thienylpyrazolecarboxamides and agrochemical fungicides containing them
INVENTOR(S): Yoshikawa, Yukihiro; Tomitani, Kanji; Katsuta, Hiroyuki; Kawashima, Hideo; Takahashi, Tamotsu; Inami, Shunichi; Yanase, Yuji; Takashi, Atsuo; Shimotori, Hitoshi; Tomura, Naofumi
PATENT ASSIGNEE(S): Mitsui Toatsu Chemicals, Inc., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 51 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 09301974	A2	19971125	JP 1996-121387	19960516

PRIORITY APPLN. INFO.: JP 1996-121387 19960516
OTHER SOURCE(S): MARPAT 128:22908
GI



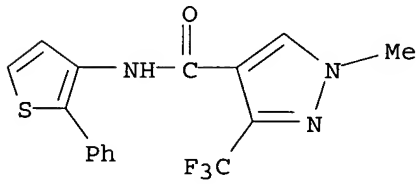
I

AB The title compds. I (Q = H, Me, CF3, F, Cl, Br, iodine, MeO, MeS, MeSO3, MeSO2, cyano, Ac, NO2, alkoxycarbonyl, NH2; R = C1-12 linear or branched (halo)alkyl, C2-10 linear or branched (halo)alkenyl, C2-10 alkylthioalkyl, C2-10 alkoxyalkyl, C3-10 cyclo(halo)alkyl, (un)substituted Ph; R1 = CF3, CHF2, Me, Et, Cl, Br, iodine) are prepared 2-Nitro-3-(4-tolyl)thiophene was subjected to catalytic hydrogenation over Pd/C at room temperature for 5 h in dioxane, filtered, and the filtrate was treated with pyridine and 3-trifluoromethyl-1-methylpyrazole-4-carbonyl chloride at room temperature for 1

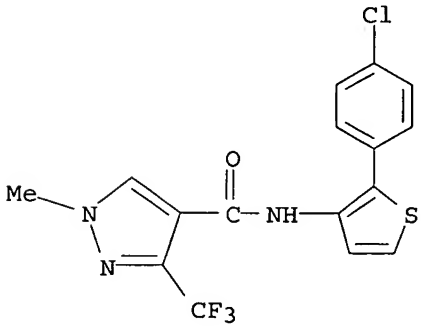
h to give 47% N-[2-[3-(4-tolyl)]thienyl]-3-trifluoromethyl-1-methylpyrazole-4-carboxamide, which showed 70% antifungal activity.

IT **183675-93-6P 183675-95-8P 183675-99-2P**
183676-07-5P 183676-11-1P 183676-13-3P
183676-14-4P 183676-15-5P 183676-16-6P
183676-17-7P 183676-18-8P 183676-19-9P
183676-20-2P 183676-24-6P 183676-25-7P
183676-26-8P 183676-27-9P 183676-28-0P
183676-29-1P 183676-30-4P 183676-31-5P
183676-32-6P 183676-41-7P 183676-42-8P
183676-44-0P 183676-45-1P 183676-49-5P
183676-50-8P 183676-51-9P 183676-52-0P
183676-53-1P 183676-54-2P 183676-55-3P
183676-56-4P 183676-57-5P 183676-58-6P
183676-64-4P 183676-66-6P 183721-96-2P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of N-thienylpyrazolecarboxamides as agrochem. fungicides)

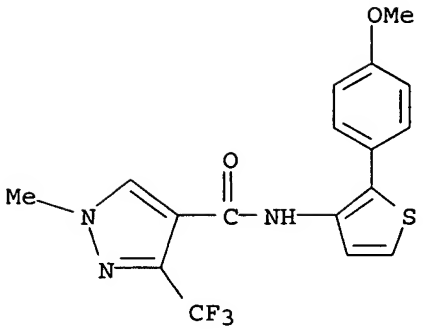
RN 183675-93-6 CAPLUS
CN 1H-Pyrazole-4-carboxamide, 1-methyl-N-(2-phenyl-3-thienyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



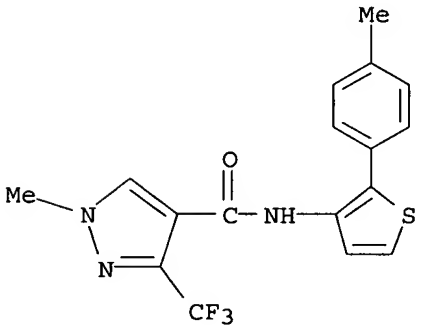
RN 183675-95-8 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[2-(4-chlorophenyl)-3-thienyl]-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



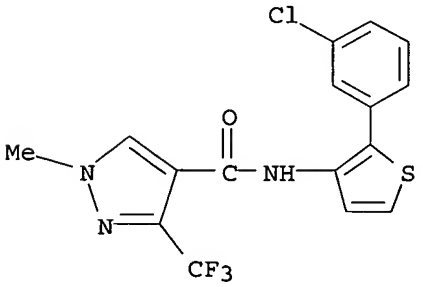
RN 183675-99-2 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[2-(4-methoxyphenyl)-3-thienyl]-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



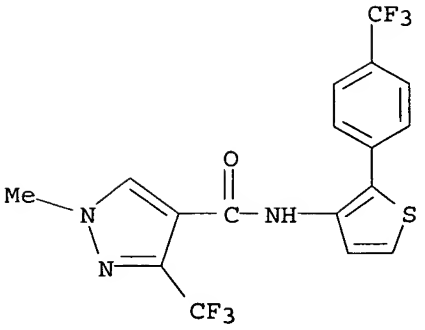
RN 183676-07-5 CAPLUS
CN 1H-Pyrazole-4-carboxamide, 1-methyl-N-[2-(4-methylphenyl)-3-thienyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



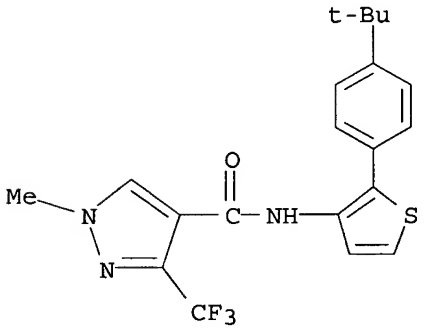
RN 183676-11-1 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[2-(3-chlorophenyl)-3-thienyl]-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



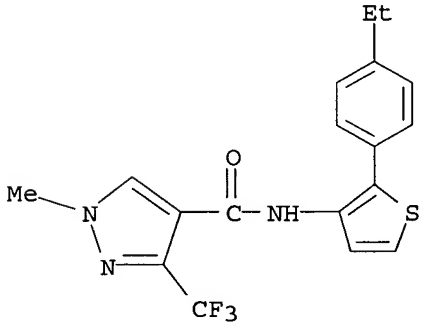
RN 183676-13-3 CAPLUS
CN 1H-Pyrazole-4-carboxamide, 1-methyl-3-(trifluoromethyl)-N-[2-[4-(trifluoromethyl)phenyl]-3-thienyl]- (9CI) (CA INDEX NAME)



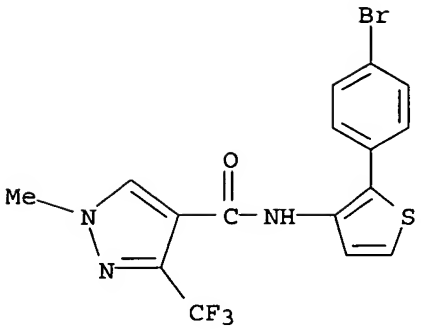
RN 183676-14-4 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[2-[4-(1,1-dimethylethyl)phenyl]-3-thienyl]-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



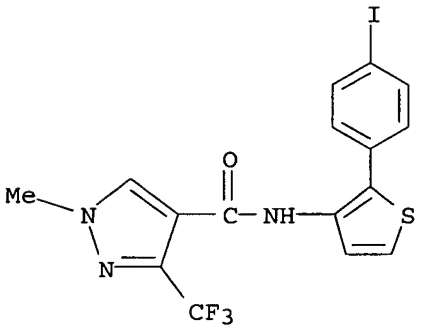
RN 183676-15-5 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[2-(4-ethylphenyl)-3-thienyl]-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



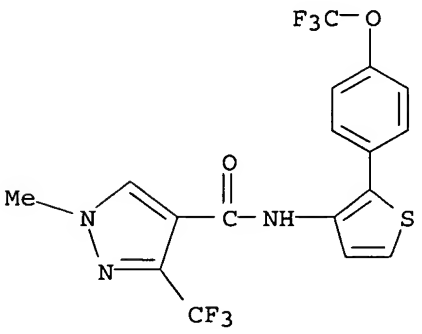
RN 183676-16-6 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[2-(4-bromophenyl)-3-thienyl]-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



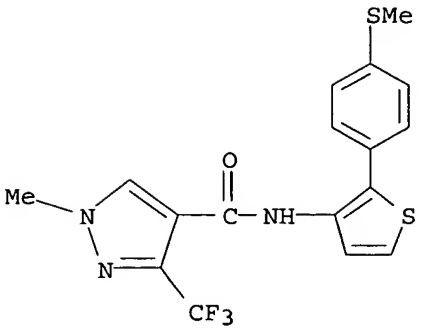
RN 183676-17-7 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[2-(4-iodophenyl)-3-thienyl]-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



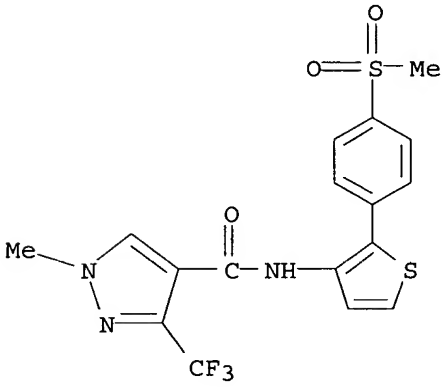
RN 183676-18-8 CAPLUS
CN 1H-Pyrazole-4-carboxamide, 1-methyl-N-[2-[4-(trifluoromethoxy)phenyl]-3-thienyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



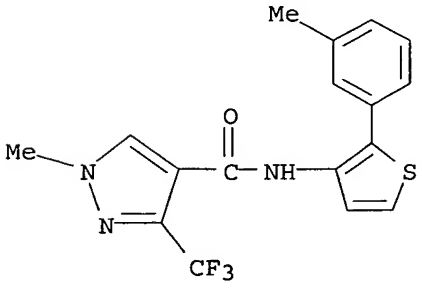
RN 183676-19-9 CAPLUS
CN 1H-Pyrazole-4-carboxamide, 1-methyl-N-[2-[4-(methylthio)phenyl]-3-thienyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



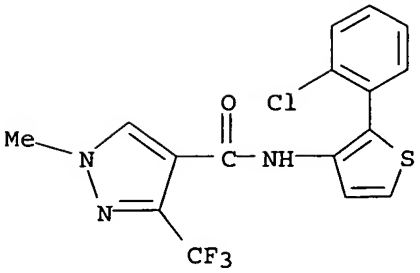
RN 183676-20-2 CAPLUS
CN 1H-Pyrazole-4-carboxamide, 1-methyl-N-[2-[4-(methylsulfonyl)phenyl]-3-thienyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



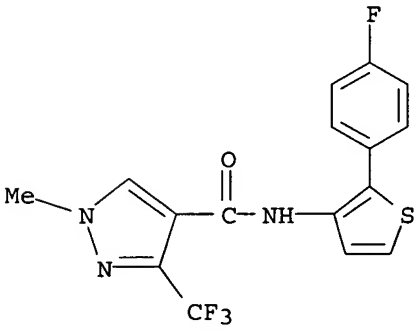
RN 183676-24-6 CAPLUS
CN 1H-Pyrazole-4-carboxamide, 1-methyl-N-[2-(3-methylphenyl)-3-thienyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



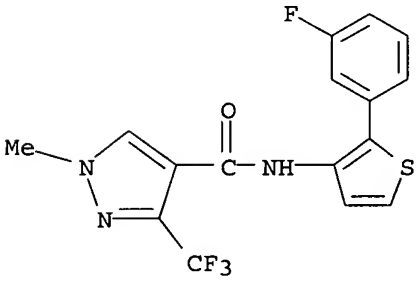
RN 183676-25-7 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[2-(2-chlorophenyl)-3-thienyl]-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



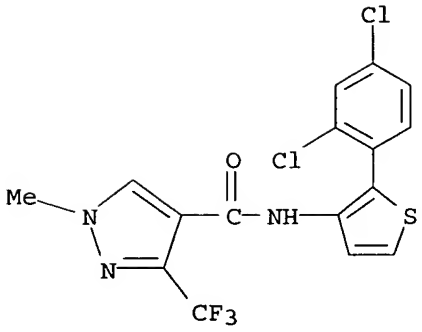
RN 183676-26-8 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[2-(4-fluorophenyl)-3-thienyl]-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



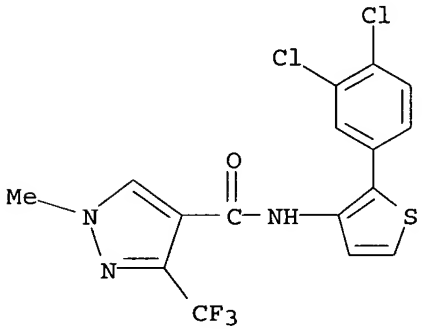
RN 183676-27-9 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[2-(3-fluorophenyl)-3-thienyl]-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



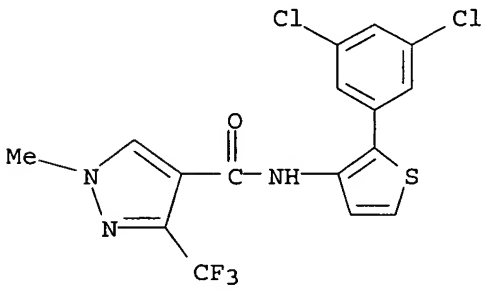
RN 183676-28-0 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[2-(2,4-dichlorophenyl)-3-thienyl]-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



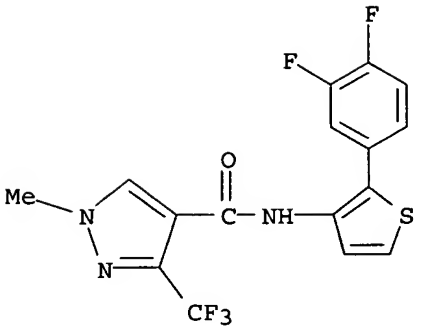
RN 183676-29-1 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[2-(3,4-dichlorophenyl)-3-thienyl]-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



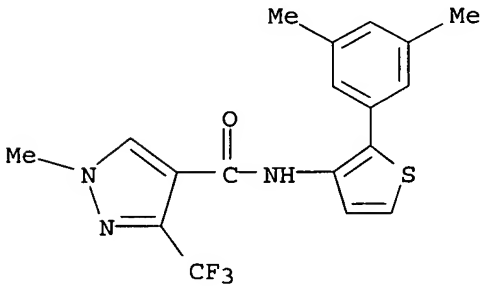
RN 183676-30-4 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[2-(3,5-dichlorophenyl)-3-thienyl]-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



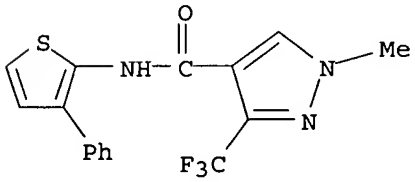
RN 183676-31-5 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[2-(3,4-difluorophenyl)-3-thienyl]-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



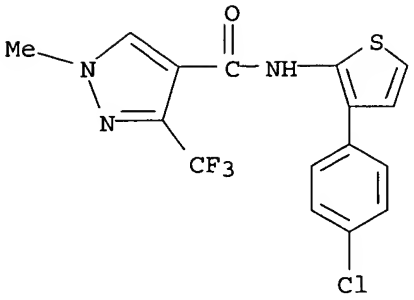
RN 183676-32-6 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[2-(3,5-dimethylphenyl)-3-thienyl]-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



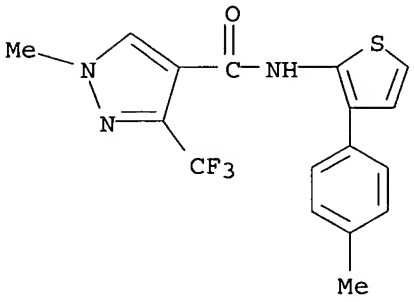
RN 183676-41-7 CAPLUS
CN 1H-Pyrazole-4-carboxamide, 1-methyl-N-(3-phenyl-2-thienyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



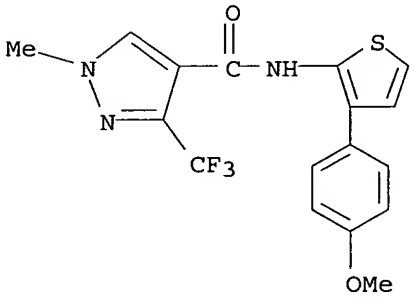
RN 183676-42-8 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[3-(4-chlorophenyl)-2-thienyl]-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



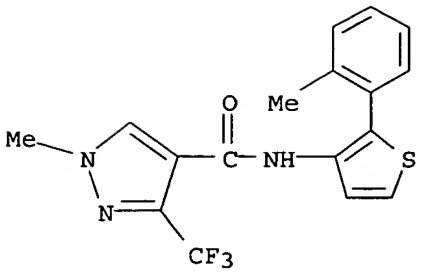
RN 183676-44-0 CAPLUS
CN 1H-Pyrazole-4-carboxamide, 1-methyl-N-[3-(4-methylphenyl)-2-thienyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



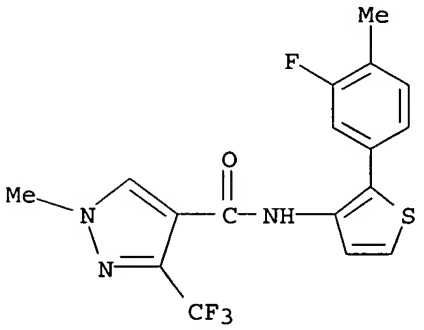
RN 183676-45-1 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[3-(4-methoxyphenyl)-2-thienyl]-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



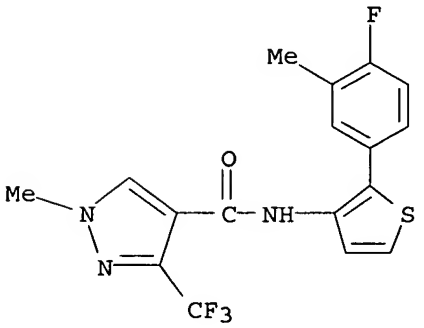
RN 183676-49-5 CAPLUS
CN 1H-Pyrazole-4-carboxamide, 1-methyl-N-[2-(2-methylphenyl)-3-thienyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



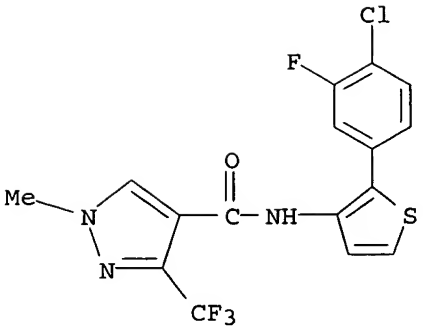
RN 183676-50-8 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[2-(3-fluoro-4-methylphenyl)-3-thienyl]-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



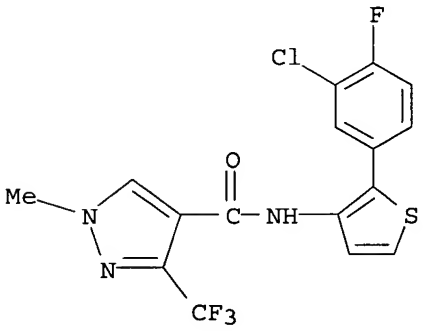
RN 183676-51-9 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[2-(4-fluoro-3-methylphenyl)-3-thienyl]-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



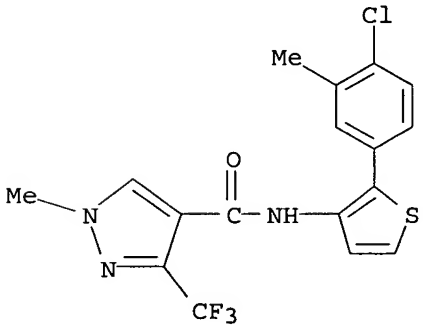
RN 183676-52-0 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[2-(4-chloro-3-fluorophenyl)-3-thienyl]-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



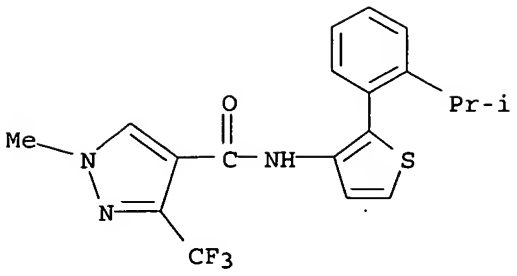
RN 183676-53-1 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[2-(3-chloro-4-fluorophenyl)-3-thienyl]-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



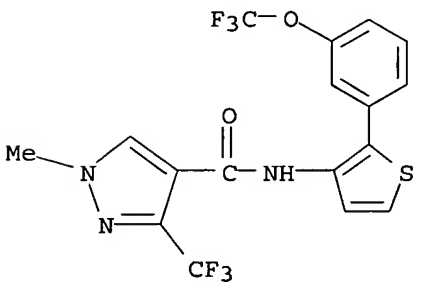
RN 183676-54-2 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[2-(4-chloro-3-methylphenyl)-3-thienyl]-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



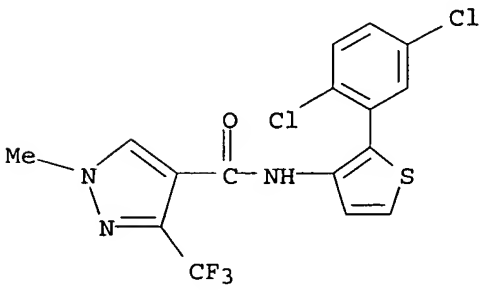
RN 183676-55-3 CAPLUS
CN 1H-Pyrazole-4-carboxamide, 1-methyl-N-[2-[2-(1-methylethyl)phenyl]-3-thienyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



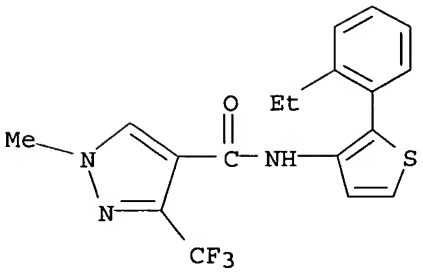
RN 183676-56-4 CAPLUS
CN 1H-Pyrazole-4-carboxamide, 1-methyl-N-[2-[3-(trifluoromethoxy)phenyl]-3-thienyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



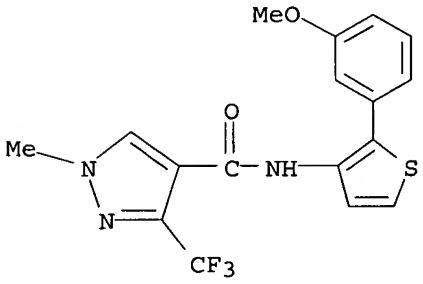
RN 183676-57-5 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[2-(2,5-dichlorophenyl)-3-thienyl]-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



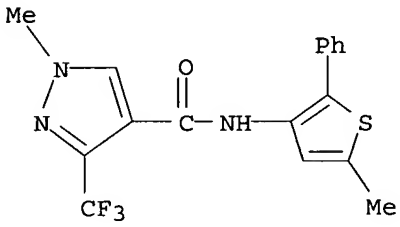
RN 183676-58-6 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[2-(2-ethylphenyl)-3-thienyl]-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



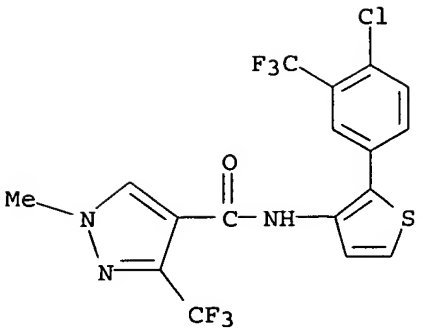
RN 183676-64-4 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[2-(3-methoxyphenyl)-3-thienyl]-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 183676-66-6 CAPLUS
CN 1H-Pyrazole-4-carboxamide, 1-methyl-N-(5-methyl-2-phenyl-3-thienyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



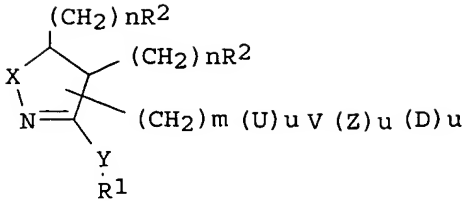
RN 183721-96-2 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[2-[4-chloro-3-(trifluoromethyl)phenyl]-3-thienyl]-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



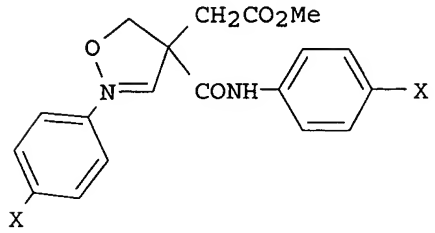
L18 ANSWER 16 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:503386 CAPLUS
DOCUMENT NUMBER: 127:135788
TITLE: Preparation of isoxazoline, isothiazoline and pyrazoline as factor Xa inhibitors
INVENTOR(S): Quan, Mimi Lifen; Wityak, John; Galemmo, Robert Anthony, Jr.; Stouten, Petrus F. W.; Pruitt, James Russell
PATENT ASSIGNEE(S): Du Pont Merck Pharmaceutical Company, USA
SOURCE: PCT Int. Appl., 191 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 9723212	A1	19970703	WO 1996-US20076		19961217
W: AM, AU, AZ, BR, BY, CA, CN, CZ, EE, HU, IL, JP, KG, KR, KZ, LT, LV, MD, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, UA, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM					
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE					
CA 2240946	AA	19970703	CA 1996-2240946		19961217
CA 2240946	C	20020910			
AU 9713358	A1	19970717	AU 1997-13358		19961217
EP 874629	A1	19981104	EP 1996-944844		19961217
EP 874629	B1	20040519			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI					
US 5939418	A	19990817	US 1996-768908		19961217
JP 2001502655	T2	20010227	JP 1997-523762		19961217
AT 267011	E	20040615	AT 1996-944844		19961217
ES 2219706	T3	20041201	ES 1996-944844		19961217
ZA 9610704	A	19980619	ZA 1996-10704		19961219
PRIORITY APPLN. INFO.:			US 1995-9508P	P	19951221
			US 1996-646903	A	19960508
			US 1996-30666P	P	19961112
			WO 1996-US20076	W	19961217

OTHER SOURCE(S): MARPAT 127:135788
GI



I



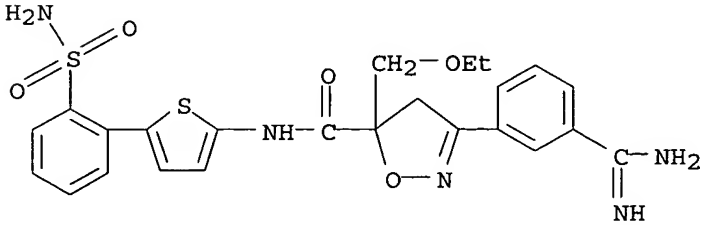
II

AB The title compds. [I; U = CONH(CH2)o, CO(CH2)o, SO2NH(CH2)o, etc.; o = 0-2; X = O, S, etc.; Y = (un)substituted aryl or heteroaryl, etc.; R1 = (CH2)pNR5R6, CONR5R6, etc.; R5, R6 = H, C1-6 alkyl, etc.; R2 = H, C1-6 alkyl or alkoxy, COR5, etc.; U, R2 = may combine together to provide a spiro compound of heterocycle; V = (un)substituted aryl or heteroaryl, etc.; Z = CO, single bond, NH, O, etc.; D = (un)substituted aryl or heteroaryl, etc.; u = 0-1; m = 0-2; n = 0-4] are prepared I, possessing Factor Xa inhibitory activity, are useful as anticoagulant agents for treatment and prevention of thromboembolic disorders (no data). Thus, isoxazoline derivative (II; X = CN) (preparation given) was treated with HCl gas and then reacted with NH4OAc. The reaction mixture was purified by HPLC eluted with F3CCO2H (TFA) to give 20% the title compound II.3TFA (X = NH2C:NH).

IT **193005-98-0P 193005-99-1P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of isoxazoline, isothiazoline and pyrazoline as factor Xa inhibitors)

RN 193005-98-0 CAPLUS

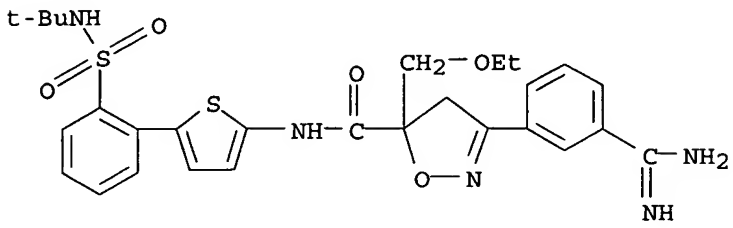
CN 5-Isoxazolecarboxamide, 3-[3-(aminoiminomethyl)phenyl]-N-[5-[2-(aminosulfonyl)phenyl]-2-thienyl]-5-(ethoxymethyl)-4,5-dihydro- (9CI) (CA INDEX NAME)



RN 193005-99-1 CAPLUS

CN 5-Isoxazolecarboxamide, 3-[3-(aminoiminomethyl)phenyl]-N-[5-[2-[[(1,1-

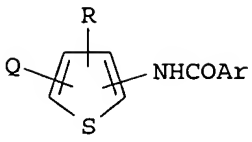
dimethylethyl)amino]sulfonyl]phenyl]-2-thienyl]-5-(ethoxymethyl)-4,5-dihydro- (9CI) (CA INDEX NAME)



L18 ANSWER 17 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1996:718179 CAPLUS
DOCUMENT NUMBER: 126:7982
TITLE: Preparation of thiophene derivative as agricultural and horticultural fungicides
INVENTOR(S): Yoshikawa, Yukihiro; Tomiya, Kanji; Katsuta, Hiroyuki; Kawashima, Hideo; Takahashi, Osamu; Inami, Shunichi; Yanase, Yuji; Kishi, Junro; Shimotori, Hitoshi; Tomura, Naofumi
PATENT ASSIGNEE(S): Mitsui Toatsu Chemicals, Incorporated, Japan
SOURCE: Eur. Pat. Appl., 59 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 737682	A1	19961016	EP 1996-105345	19960403
EP 737682	B1	20020109		
R: CH, DE, ES, FR, GB, IT, LI				
US 5747518	A	19980505	US 1996-627929	19960403
ES 2169773	T3	20020716	ES 1996-105345	19960403
CA 2173788	AA	19961012	CA 1996-2173788	19960410
CA 2173788	C	20001128		
JP 09235282	A2	19970909	JP 1996-88259	19960410
JP 3164762	B2	20010508		
KR 201426	B1	19990615	KR 1996-10708	19960410
JP 2001151770	A2	20010605	JP 2000-320150	19960410
JP 3385264	B2	20030310		
CN 1146993	A	19970409	CN 1996-108007	19960411
CN 1061657	B	20010207		

PRIORITY APPLN. INFO.: JP 1995-85601 A 19950411
JP 1995-340480 A 19951227
JP 1996-88259 A3 19960410
OTHER SOURCE(S): MARPAT 126:7982
GI



I

AB The title compds. [I; Q = H, F, Cl, Br, iodo, Me, CF3, MeO, MeS, MeSO2, cyano, COMe, NO2, NH2, alkoxycarbonyl; R = linear or branched C1-12 (halo)alkyl or (halo)alkenyl, alkoxyalkyl, (un)substituted Ph, C2-4 alkynyl, etc.; R and NHCOAr are adjacent to each other; Ar = substituted 5-thiazolyl, N-methyl-4-pyrazolyl, 3-furyl, 2- or 3-thiophenyl, Ph, 2-chloro-3-pyridyl, or 2-pyrazinyl] are prepared I are useful for controlling plant diseases such as gray mold (Botrytis cinerea), and powdery mildew (Erysiphe cichoracearum), and as fungicides for resistant fungus, and pathogenic fungus of various crops. Thus, N-(2-isopropenyl-3-thienyl)-3-trifluoromethyl-1-methylpyrazole-4-carboxamide (preparation given) was hydrogenated over 5% Pd/C to give 79% I (Q = H, R = 2-i-Pr, Ar = N-methyl-3-trifluoromethylpyrazol-4-yl) (II). II at 100 ppm prevented 100% infection of kidney beans seedlings with gray mold (RS or RR strain), powdery mildew (EBI resistant), and rust (EBI sensitive).

IT **183675-93-6P 183675-95-8P 183675-97-0P**
183675-99-2P 183676-03-1P 183676-05-3P
183676-07-5P 183676-09-7P 183676-11-1P
183676-12-2P 183676-13-3P 183676-14-4P
183676-15-5P 183676-16-6P 183676-17-7P
183676-18-8P 183676-19-9P 183676-20-2P
183676-22-4P 183676-24-6P 183676-25-7P
183676-26-8P 183676-27-9P 183676-28-0P
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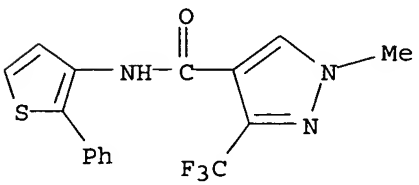
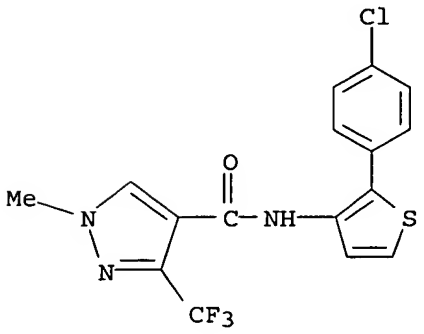
183676-49-5P 183676-50-8P 183676-51-9P
183676-52-0P 183676-53-1P 183676-54-2P
183676-55-3P 183676-56-4P 183676-57-5P
183676-58-6P 183676-59-7P 183676-61-1P
183676-62-2P 183676-63-3P 183676-64-4P
183676-65-5P 183676-66-6P 183721-96-2P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of thiophene derivative as agricultural and horticultural fungicides)

RN 183675-93-6 CAPLUS

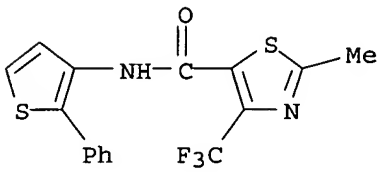
CN 1H-Pyrazole-4-carboxamide, 1-methyl-N-(2-phenyl-3-thienyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



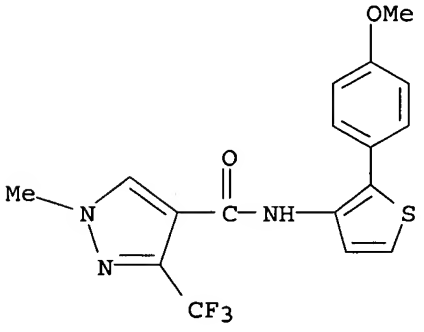
RN 183675-95-8 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[2-(4-chlorophenyl)-3-thienyl]-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



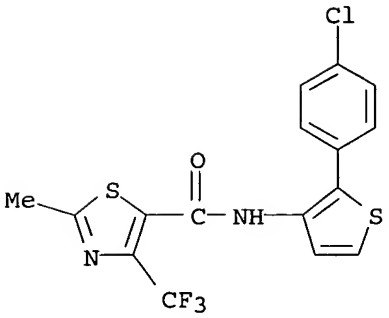
RN 183675-97-0 CAPLUS
CN 5-Thiazolecarboxamide, 2-methyl-N-(2-phenyl-3-thienyl)-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)



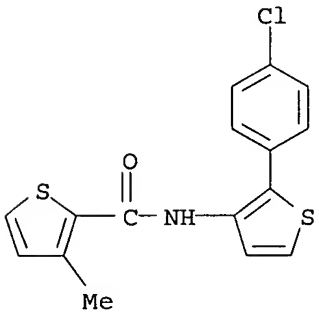
RN 183675-99-2 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[2-(4-methoxyphenyl)-3-thienyl]-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



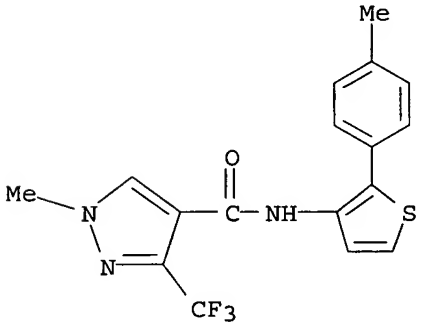
RN 183676-03-1 CAPLUS
CN 5-Thiazolecarboxamide, N-[2-(4-chlorophenyl)-3-thienyl]-2-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)



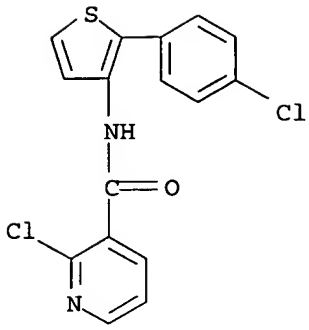
RN 183676-05-3 CAPLUS
CN 2-Thiophenecarboxamide, N-[2-(4-chlorophenyl)-3-thienyl]-3-methyl- (9CI) (CA INDEX NAME)



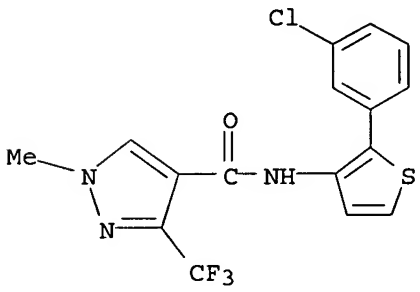
RN 183676-07-5 CAPLUS
CN 1H-Pyrazole-4-carboxamide, 1-methyl-N-[2-(4-methylphenyl)-3-thienyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



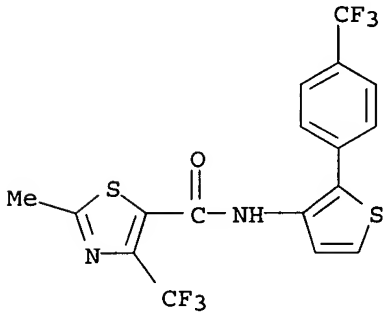
RN 183676-09-7 CAPLUS
CN 3-Pyridinecarboxamide, 2-chloro-N-[2-(4-chlorophenyl)-3-thienyl]- (9CI) (CA INDEX NAME)



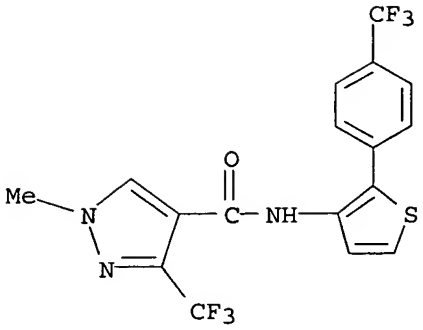
RN 183676-11-1 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[2-(3-chlorophenyl)-3-thienyl]-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



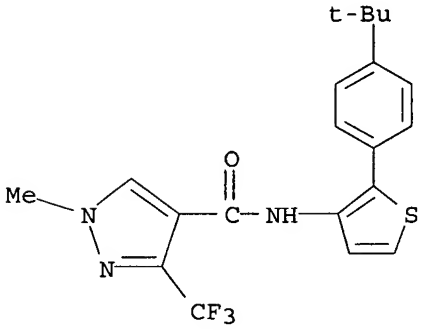
RN 183676-12-2 CAPLUS
CN 5-Thiazolecarboxamide, 2-methyl-4-(trifluoromethyl)-N-[2-[4-(trifluoromethyl)phenyl]-3-thienyl]- (9CI) (CA INDEX NAME)



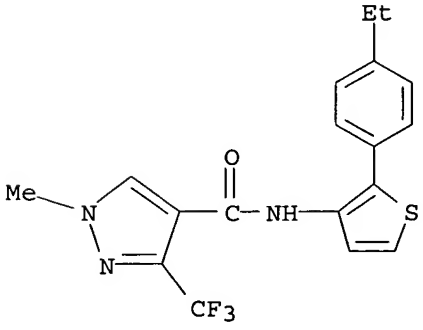
RN 183676-13-3 CAPLUS
CN 1H-Pyrazole-4-carboxamide, 1-methyl-3-(trifluoromethyl)-N-[2-[4-(trifluoromethyl)phenyl]-3-thienyl]- (9CI) (CA INDEX NAME)



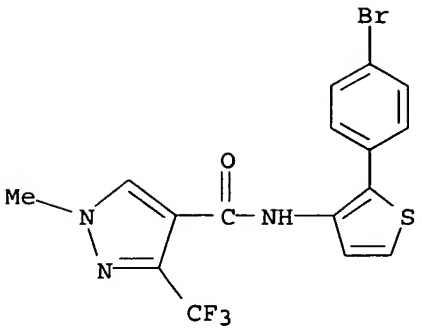
RN 183676-14-4 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[2-[4-(1,1-dimethylethyl)phenyl]-3-thienyl]-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



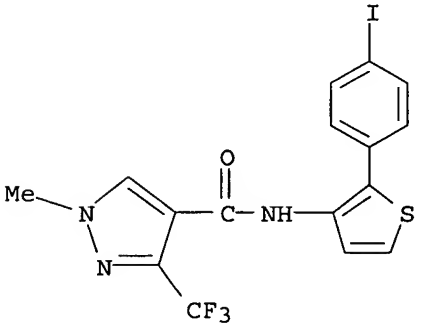
RN 183676-15-5 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[2-(4-ethylphenyl)-3-thienyl]-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



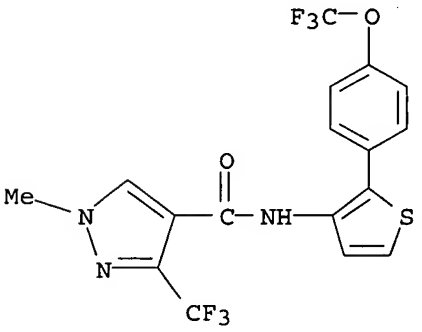
RN 183676-16-6 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[2-(4-bromophenyl)-3-thienyl]-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



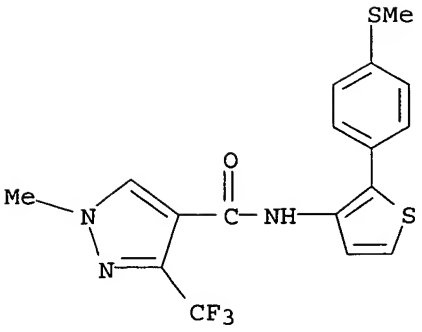
RN 183676-17-7 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[2-(4-iodophenyl)-3-thienyl]-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



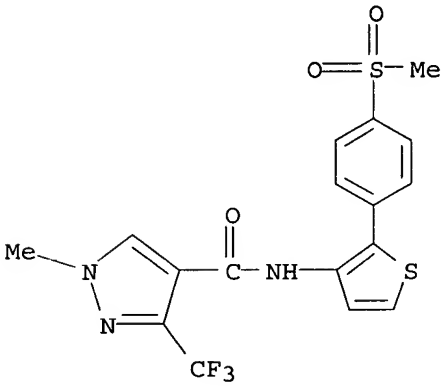
RN 183676-18-8 CAPLUS
CN 1H-Pyrazole-4-carboxamide, 1-methyl-N-[2-[4-(trifluoromethoxy)phenyl]-3-thienyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



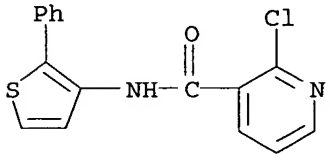
RN 183676-19-9 CAPLUS
CN 1H-Pyrazole-4-carboxamide, 1-methyl-N-[2-[4-(methylthio)phenyl]-3-thienyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



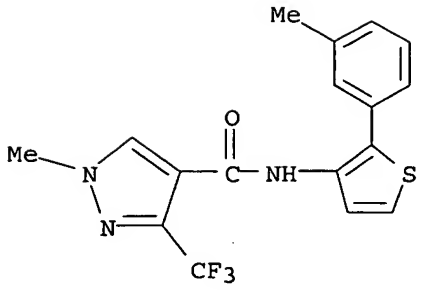
RN 183676-20-2 CAPLUS
CN 1H-Pyrazole-4-carboxamide, 1-methyl-N-[2-[4-(methylsulfonyl)phenyl]-3-thienyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



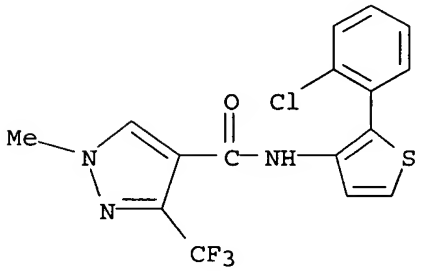
RN 183676-22-4 CAPLUS
CN 3-Pyridinecarboxamide, 2-chloro-N-(2-phenyl-3-thienyl)- (9CI) (CA INDEX NAME)



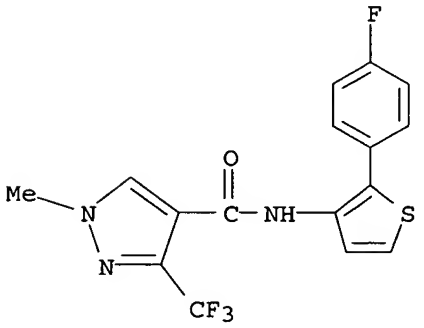
RN 183676-24-6 CAPLUS
CN 1H-Pyrazole-4-carboxamide, 1-methyl-N-[2-(3-methylphenyl)-3-thienyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



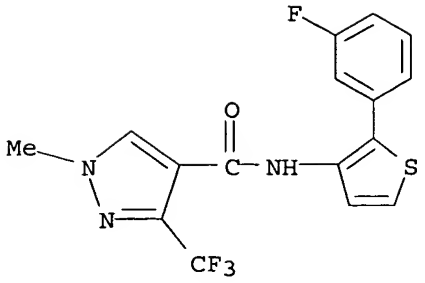
RN 183676-25-7 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[2-(2-chlorophenyl)-3-thienyl]-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



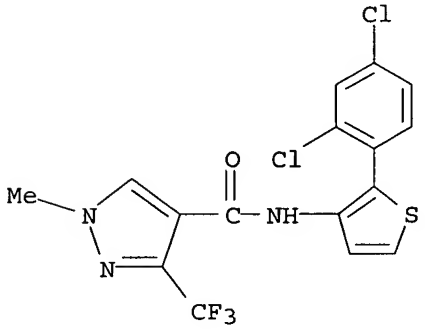
RN 183676-26-8 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[2-(4-fluorophenyl)-3-thienyl]-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



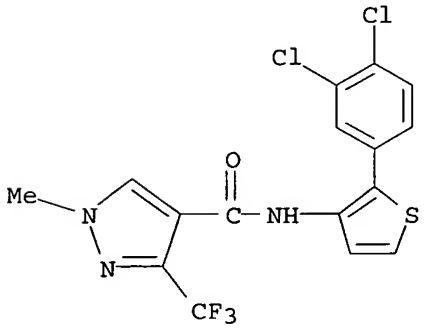
RN 183676-27-9 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[2-(3-fluorophenyl)-3-thienyl]-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



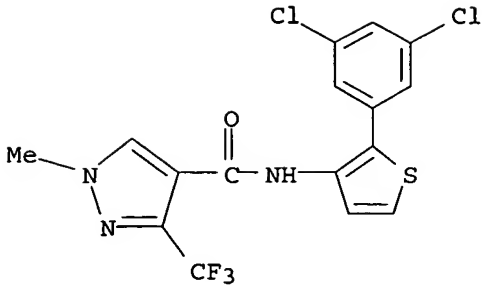
RN 183676-28-0 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[2-(2,4-dichlorophenyl)-3-thienyl]-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



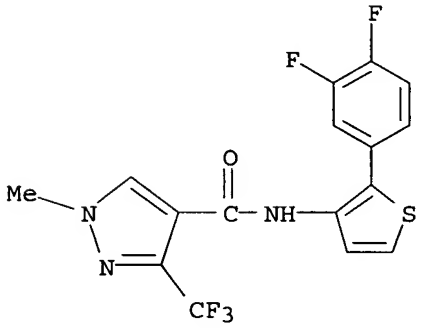
RN 183676-29-1 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[2-(3,4-dichlorophenyl)-3-thienyl]-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



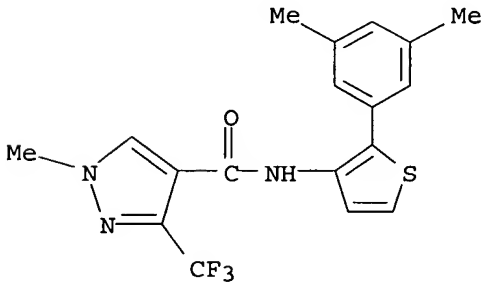
RN 183676-30-4 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[2-(3,5-dichlorophenyl)-3-thienyl]-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



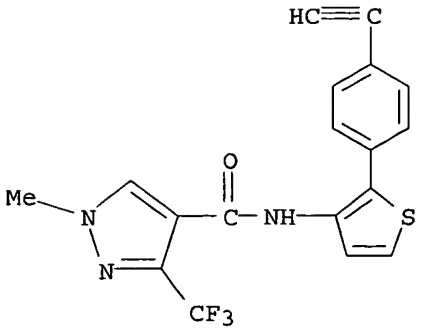
RN 183676-31-5 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[2-(3,4-difluorophenyl)-3-thienyl]-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



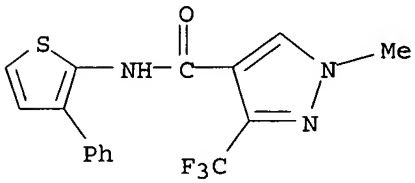
RN 183676-32-6 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[2-(3,5-dimethylphenyl)-3-thienyl]-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



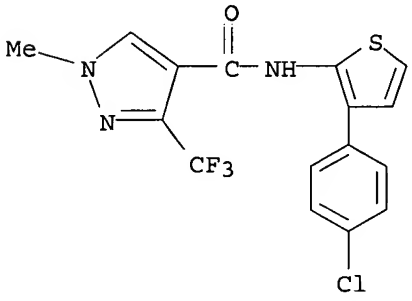
RN 183676-33-7 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[2-(4-ethynylphenyl)-3-thienyl]-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



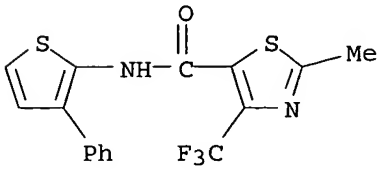
RN 183676-41-7 CAPLUS
CN 1H-Pyrazole-4-carboxamide, 1-methyl-N-(3-phenyl-2-thienyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



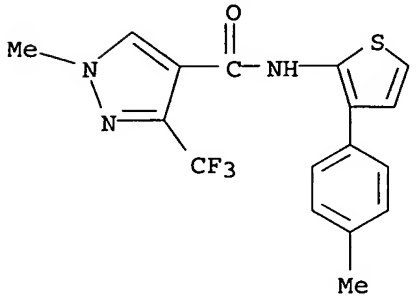
RN 183676-42-8 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[3-(4-chlorophenyl)-2-thienyl]-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



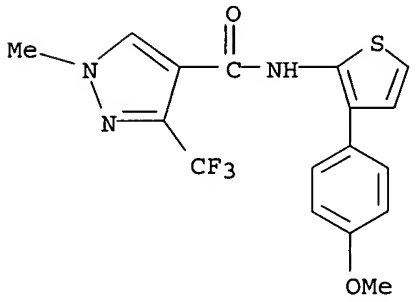
RN 183676-43-9 CAPLUS
CN 5-Thiazolecarboxamide, 2-methyl-N-(3-phenyl-2-thienyl)-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)



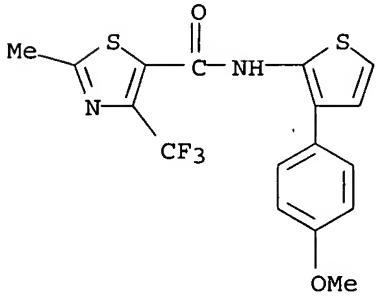
RN 183676-44-0 CAPLUS
CN 1H-Pyrazole-4-carboxamide, 1-methyl-N-[3-(4-methylphenyl)-2-thienyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



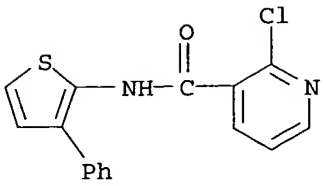
RN 183676-45-1 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[3-(4-methoxyphenyl)-2-thienyl]-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



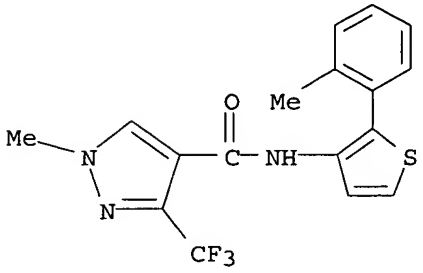
RN 183676-46-2 CAPLUS
CN 5-Thiazolecarboxamide, N-[3-(4-methoxyphenyl)-2-thienyl]-2-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)



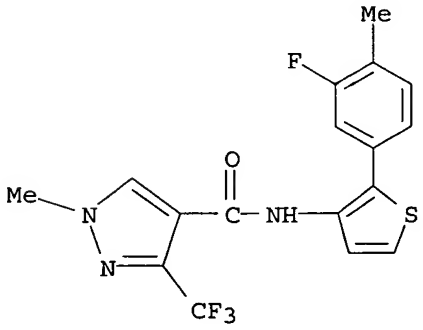
RN 183676-47-3 CAPLUS
CN 3-Pyridinecarboxamide, 2-chloro-N-(3-phenyl-2-thienyl)- (9CI) (CA INDEX NAME)



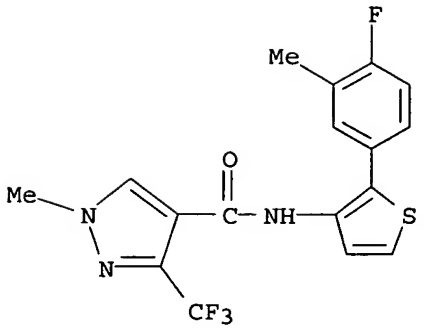
RN 183676-49-5 CAPLUS
CN 1H-Pyrazole-4-carboxamide, 1-methyl-N-[2-(2-methylphenyl)-3-thienyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



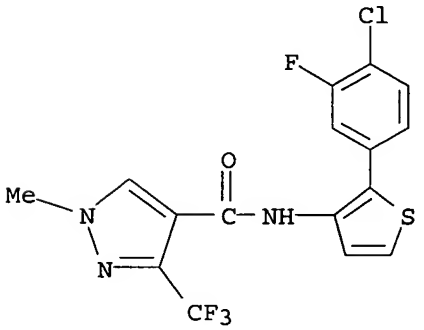
RN 183676-50-8 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[2-(3-fluoro-4-methylphenyl)-3-thienyl]-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



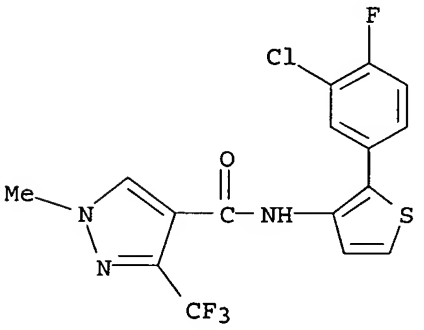
RN 183676-51-9 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[2-(4-fluoro-3-methylphenyl)-3-thienyl]-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



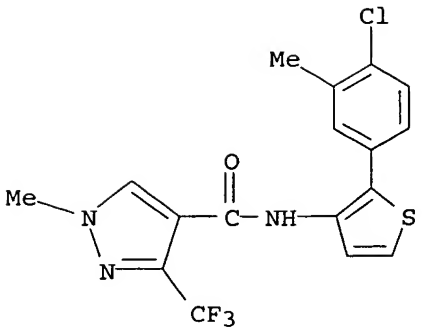
RN 183676-52-0 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[2-(4-chloro-3-fluorophenyl)-3-thienyl]-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



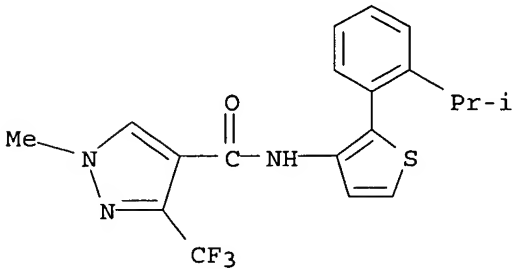
RN 183676-53-1 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[2-(3-chloro-4-fluorophenyl)-3-thienyl]-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



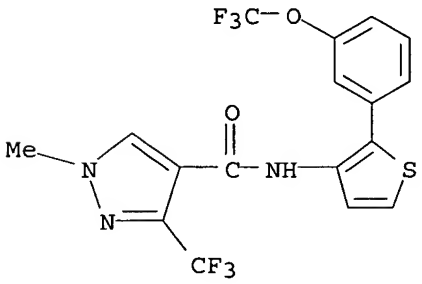
RN 183676-54-2 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[2-(4-chloro-3-methylphenyl)-3-thienyl]-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



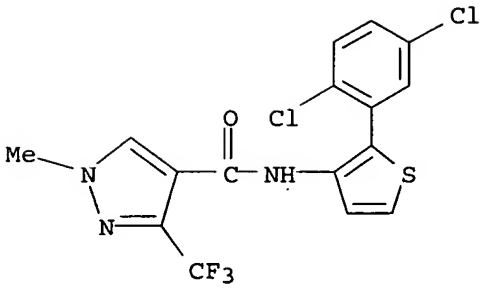
RN 183676-55-3 CAPLUS
CN 1H-Pyrazole-4-carboxamide, 1-methyl-N-[2-[2-(1-methylethyl)phenyl]-3-thienyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



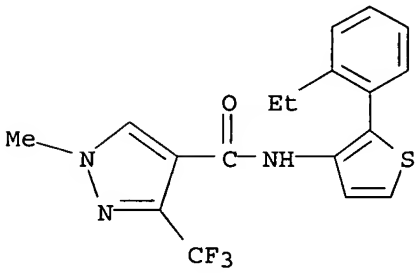
RN 183676-56-4 CAPLUS
CN 1H-Pyrazole-4-carboxamide, 1-methyl-N-[2-[3-(trifluoromethoxy)phenyl]-3-thienyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



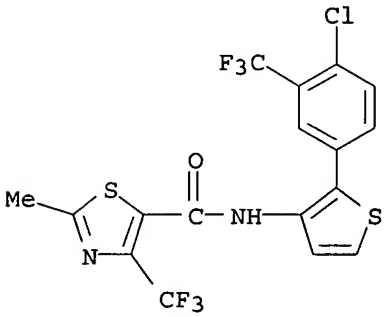
RN 183676-57-5 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[2-(2,5-dichlorophenyl)-3-thienyl]-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



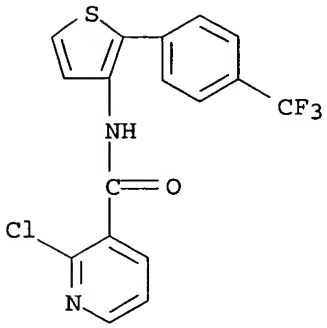
RN 183676-58-6 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[2-(2-ethylphenyl)-3-thienyl]-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



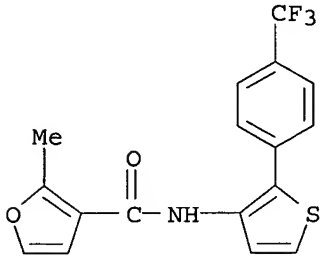
RN 183676-59-7 CAPLUS
CN 5-Thiazolecarboxamide, N-[2-[4-chloro-3-(trifluoromethyl)phenyl]-3-thienyl]-2-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)



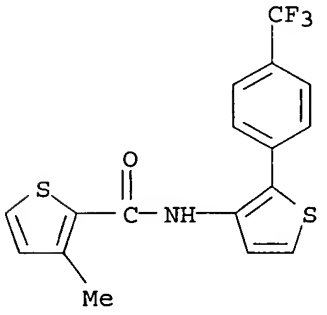
RN 183676-61-1 CAPLUS
CN 3-Pyridinecarboxamide, 2-chloro-N-[2-[4-(trifluoromethyl)phenyl]-3-thienyl]- (9CI) (CA INDEX NAME)



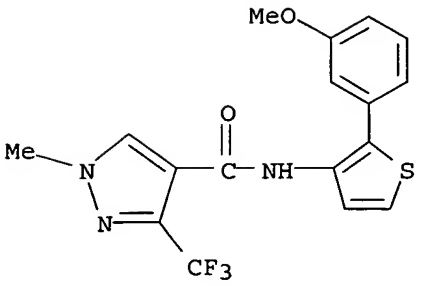
RN 183676-62-2 CAPLUS
CN 3-Furancarboxamide, 2-methyl-N-[2-[4-(trifluoromethyl)phenyl]-3-thienyl]- (9CI) (CA INDEX NAME)



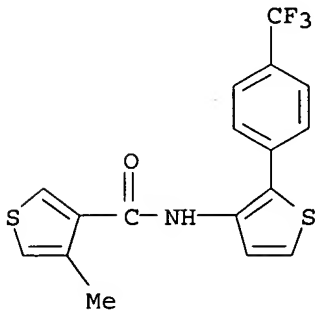
RN 183676-63-3 CAPLUS
CN 2-Thiophenecarboxamide, 3-methyl-N-[2-[4-(trifluoromethyl)phenyl]-3-thienyl]- (9CI) (CA INDEX NAME)



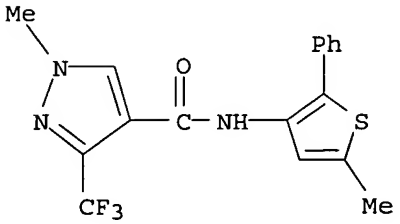
RN 183676-64-4 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[2-(3-methoxyphenyl)-3-thienyl]-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



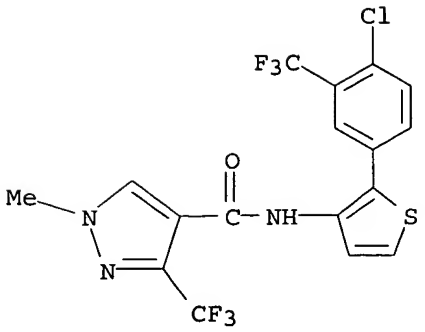
RN 183676-65-5 CAPLUS
CN 3-Thiophenecarboxamide, 4-methyl-N-[2-[4-(trifluoromethyl)phenyl]-3-thienyl]- (9CI) (CA INDEX NAME)



RN 183676-66-6 CAPLUS
CN 1H-Pyrazole-4-carboxamide, 1-methyl-N-(5-methyl-2-phenyl-3-thienyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 183721-96-2 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[2-[4-chloro-3-(trifluoromethyl)phenyl]-3-thienyl]-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



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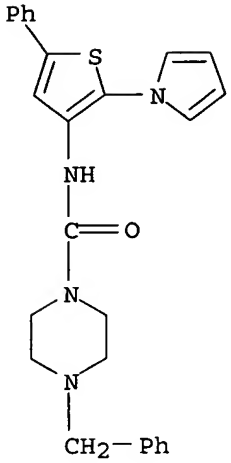
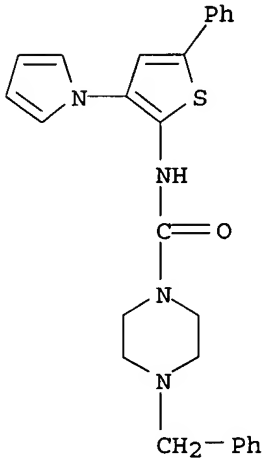
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A series of (piperazinyl)pyrrolo[1,2-a]thieno[3,2-e]pyrazines and (piperazinyl)pyrrolo[1,2-a]thieno[2,3-e]pyrazines was prepared and evaluated in order to determine the necessary requirements for high affinity on the 5-HT3 receptors and high selectivity vs. other 5-HT receptor subtypes. Various substitutions on the piperazine and the thiophene ring of the pyrrolothienopyrazine moieties were systematically explored as well as replacement of the piperazine by other cyclic amines. An example compound is 5-[4-[(4-fluorophenyl)methyl]-1-piperazinyl]pyrrolo[1,2-a]thieno[3,2-e]pyrazine trihydrochloride. These high-affinity compds. have in common a benzyl- or allylpiperazine substituent with no substitutions on the thiophene ring. Five of these compds. were evaluated on the Von Bezold-Jarisch reflex and were characterized as partial agonists. One of them, 5-[4-(phenylmethyl)-1-piperazinyl]pyrrolo[1,2-a]thieno[3,2-e]pyrazine (fumarate) was shown in vivo at very low dose a potent anxiolytic-like activity in the light/dark test.

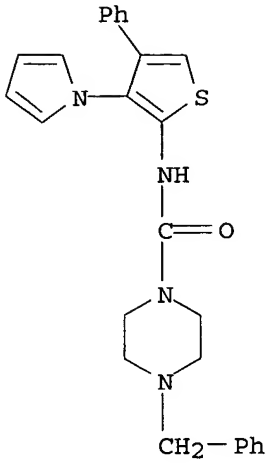
IT **153629-46-0P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(pyrrolo[1,2-a]thieno[3,2-e]pyrazines and pyrrolo[1,2-a]thieno[2,3-e]pyrazines as serotoninergic S3 neurotransmitter agonists)
RN 153629-46-0 CAPLUS
CN 1-Piperazinecarboxamide, 4-(phenylmethyl)-N-[5-phenyl-2-(1H-pyrrol-1-yl)-3-thienyl]- (9CI) (CA INDEX NAME)



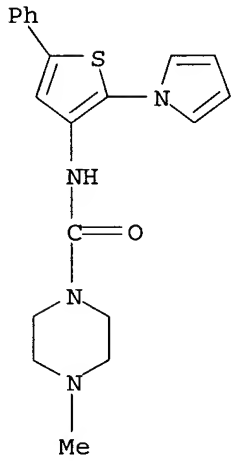
IT **153629-26-6P 153629-34-6P 153629-43-7P**
175911-96-3P 175911-98-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(pyrrolo[1,2-a]thieno[3,2-e]pyrazines and pyrrolo[1,2-a]thieno[2,3-e]pyrazines as serotoninergic S3 neurotransmitter agonists)
RN 153629-26-6 CAPLUS
CN 1-Piperazinecarboxamide, 4-(phenylmethyl)-N-[5-phenyl-3-(1H-pyrrol-1-yl)-2-thienyl]- (9CI) (CA INDEX NAME)



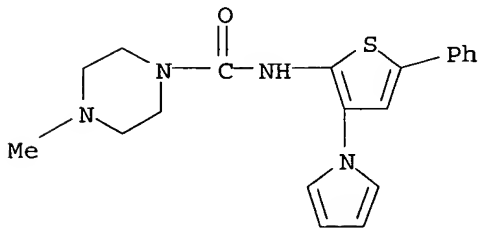
RN 153629-34-6 CAPLUS
CN 1-Piperazinecarboxamide, 4-(phenylmethyl)-N-[4-phenyl-3-(1H-pyrrol-1-yl)-2-thienyl]- (9CI) (CA INDEX NAME)



RN 153629-43-7 CAPLUS
CN 1-Piperazinecarboxamide, 4-methyl-N-[5-phenyl-2-(1H-pyrrol-1-yl)-3-thienyl]- (9CI) (CA INDEX NAME)

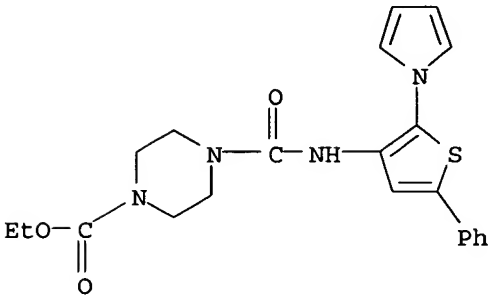


RN 175911-96-3 CAPLUS
CN 1-Piperazinecarboxamide, 4-methyl-N-[5-phenyl-3-(1H-pyrrol-1-yl)-2-thienyl]- (9CI) (CA INDEX NAME)



RN 175911-98-5 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[[[5-phenyl-2-(1H-pyrrol-1-yl)-3-

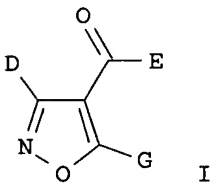
thienyl]amino]carbonyl]-, ethyl ester (9CI) (CA INDEX NAME)



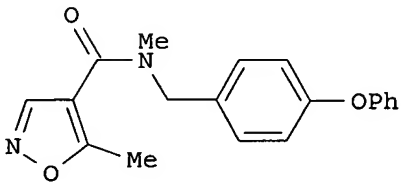
L18 ANSWER 19 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:784800 CAPLUS
DOCUMENT NUMBER: 123:285992
TITLE: Preparation of isoxazole-4-carboxylates, 2-cyano-3-hydroxyacrylates, and analogs as immunosuppressants
INVENTOR(S): Coghlan, Michael J.; Luly, Jay R.; Wiedeman, Paul E.
PATENT ASSIGNEE(S): Abbott Laboratories, USA
SOURCE: PCT Int. Appl., 99 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9424095	A1	19941027	WO 1994-US4045	19940414
W: CA, JP, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
PRIORITY APPLN. INFO.:			US 1993-48499	A 19930416
			US 1993-56500	A 19930503

OTHER SOURCE(S): MARPAT 123:285992
GI



I



II

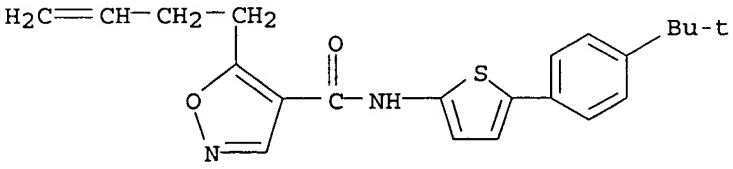
AB HOCG:C(CN)COE, GCOC(CN)COE, and isoxazoles I (D = H, alkyl, CHO, CO2H, alkoxycarbonyl, etc.; E = H, NH2, OH, Me, etc.; G = H, alkyl, Ph, etc.) were prepared Thus, prepared isoxazolecarboxamide II gave 94 and 99% inhibition of human mixed lymphocyte reaction and allogenic mixed leukocyte response, resp., at 10μM.

IT **167428-85-5P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of isoxazole-4-carboxylates, 2-cyano-3-hydroxyacrylates, and analogs as immunosuppressants)

RN 167428-85-5 CAPLUS

CN 4-Isoxazolecarboxamide, 5-(3-butenyl)-N-[5-[4-(1,1-dimethylethyl)phenyl]-2-thienyl]- (9CI) (CA INDEX NAME)



L18 ANSWER 20 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1994:217734 CAPLUS

DOCUMENT NUMBER: 120:217734

TITLE: Pyrrolothienopyrazine serotonin 5-HT3 receptor antagonists

INVENTOR(S): Rault, Sylvain; Lancelot, Jean Charles; Pilo Vincente, Juan Carlos; Robba, Max; Guardiola-Lemaitre, Beatrice; Renard, Pierre; Adam, Gerard

PATENT ASSIGNEE(S): ADIR et Compagnie, Fr.

SOURCE: Eur. Pat. Appl., 35 pp.
CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

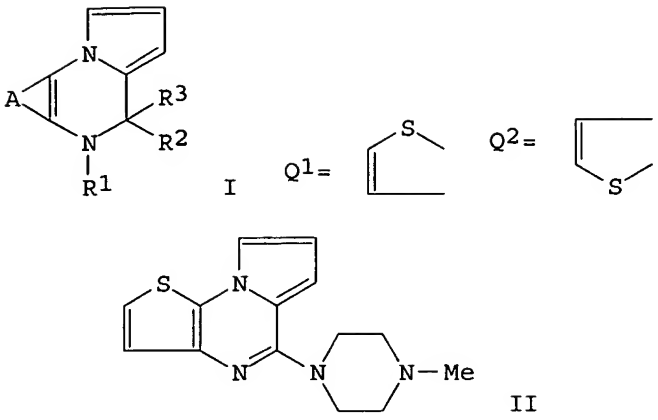
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 573360	A1	19931208	EP 1993-401416	19930603
EP 573360	B1	19980826		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
FR 2691967	A1	19931210	FR 1992-6800	19920605
FR 2691967	B1	19950609		
AT 170187	E	19980915	AT 1993-401416	19930603
ES 2123038	T3	19990101	ES 1993-401416	19930603
CA 2097779	AA	19931206	CA 1993-2097779	19930604
AU 9340059	A1	19931209	AU 1993-40059	19930604
AU 659738	B2	19950525		
ZA 9303942	A	19931230	ZA 1993-3942	19930604
JP 06172363	A2	19940621	JP 1993-134922	19930604
JP 07094460	B4	19951011		

PRIORITY APPLN. INFO.: FR 1992-6800 A 19920605

OTHER SOURCE(S): MARPAT 120:217734

GI



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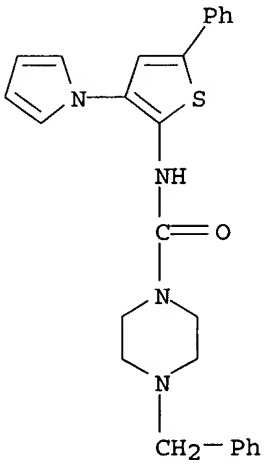
II

AB The title compds. I [A = (un)substituted Q1, (un)substituted Q2; R1R2 form a double bond and R3 represents a Cl atom, a substituted amine or heterocyclyl group, or no group or R1 may represent a H and R2R3 a :O], which are highly specific serotonin 5-HT3 receptor antagonists (no data), useful in the treatment of depression (no data), stress (no data) psychoses (no data), migraine headache (no data), etc., are prepared and I-containing formulations presented. Thus, 2-(pyrrol-1-yl)-3-thenoyl nitride was refluxed in 1,2-dichlorobenzene, the intermediate heated in the presence of POCl2, and condensed with 1-methylpiperazine, producing pyrazine II, m.p. 82°.

IT **153629-26-6 153629-34-6 153629-43-7**
153629-46-0 153629-49-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation as intermediate in preparation of pyrrolothienopyrazine serotonin
5-HT3 receptor antagonists)

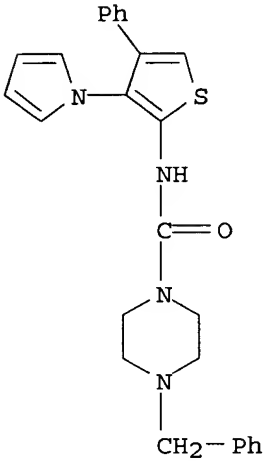
RN 153629-26-6 CAPLUS

CN 1-Piperazinecarboxamide, 4-(phenylmethyl)-N-[5-phenyl-3-(1H-pyrrol-1-yl)-2-thienyl]- (9CI) (CA INDEX NAME)

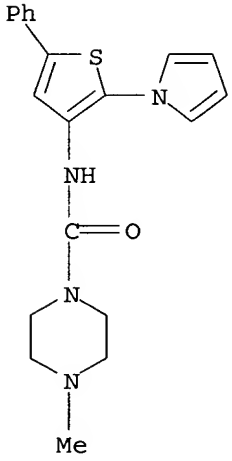


RN 153629-34-6 CAPLUS

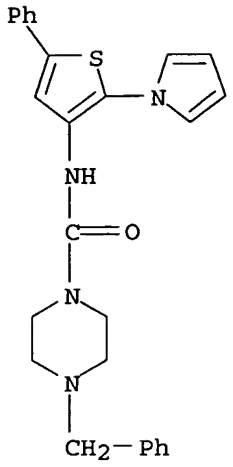
CN 1-Piperazinecarboxamide, 4-(phenylmethyl)-N-[4-phenyl-3-(1H-pyrrol-1-yl)-2-thienyl]- (9CI) (CA INDEX NAME)



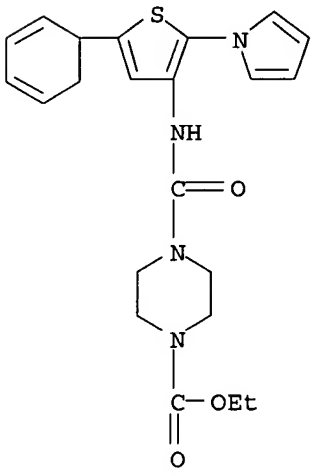
RN 153629-43-7 CAPLUS
CN 1-Piperazinecarboxamide, 4-methyl-N-[5-phenyl-2-(1H-pyrrol-1-yl)-3-thienyl]- (9CI) (CA INDEX NAME)



RN 153629-46-0 CAPLUS
CN 1-Piperazinecarboxamide, 4-(phenylmethyl)-N-[5-phenyl-2-(1H-pyrrol-1-yl)-3-thienyl]- (9CI) (CA INDEX NAME)



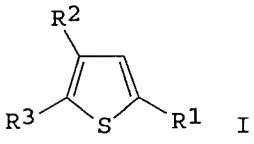
RN 153629-49-3 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[[[5-(2,4-cyclohexadien-1-yl)-2-(1H-pyrrol-1-yl)-3-thienyl]amino]carbonyl]-, ethyl ester (9CI) (CA INDEX NAME)



L18 ANSWER 21 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1992:194141 CAPLUS
DOCUMENT NUMBER: 116:194141
TITLE: Preparation of 4,5-diarylthiophenes as analgesics and antiinflammatories
INVENTOR(S): Matsuo, Masaaki; Tsuji, Kiyoshi; Konishi, Nobukiyo; Nakamura, Katsuya
PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 143 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9119708	A1	19911226	WO 1991-JP744	19910531
W: AU, CA, FI, HU, JP, KR, NO, SU, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, NL, SE				
AU 9179731	A1	19920107	AU 1991-79731	19910531
JP 06501919	T2	19940303	JP 1991-509612	19910531
EP 593761	A1	19940427	EP 1991-910169	19910531
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
ZA 9104241	A	19920325	ZA 1991-4241	19910604
CN 1059142	A	19920304	CN 1991-104746	19910610
US 5571810	A	19961105	US 1995-422545	19950413
PRIORITY APPLN. INFO.:			GB 1990-12936 A	19900611
			WO 1991-JP744 A	19910531
			US 1992-955739 B1	19921203

OTHER SOURCE(S): MARPAT 116:194141
GI



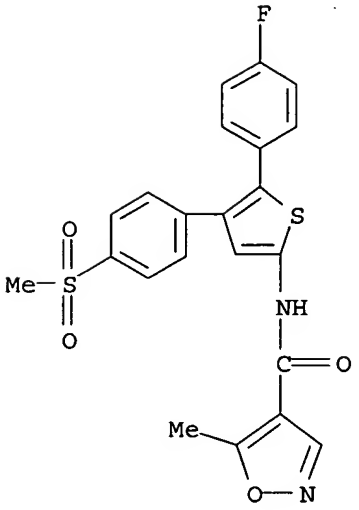
I

AB Title compds. [I; R1 = H, halo, acyl, (substituted) alkyl, alkenyl, NH2, heterocyclyl, etc.; R2, R3 = (substituted) aryl] were prepared Thus, I [R2 = 4-(MeO2S)C6H4, R3 = 4-FC6H4] (II; R1 = H) was treated sequentially with ClSO2OH and MeNH2 to give II (R1 = SO2NHMe). II (R1 = CF3) gave 87.0% inhibition of adjuvant-induced arthritis in rats at 0.1 mg/kg/day orally.

IT **140403-55-0P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as analgesic and antiinflammatory)

RN 140403-55-0 CAPLUS

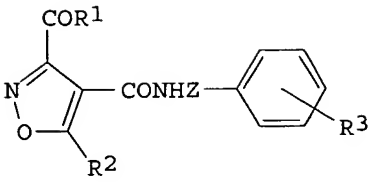
CN 4-Isoxazolecarboxamide, N-[5-(4-fluorophenyl)-4-[4-(methylsulfonyl)phenyl]-2-thienyl]-5-methyl- (9CI) (CA INDEX NAME)



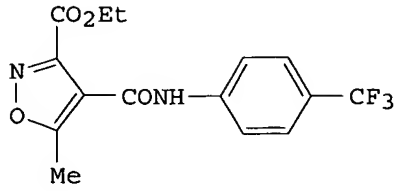
L18 ANSWER 22 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1991:559126 CAPLUS
DOCUMENT NUMBER: 115:159126
TITLE: Preparation and formulation of 3-carboxy-4-isoxazolecarboxamides as antiinflammatories and immunomodulators
INVENTOR(S): Patterson, John W.; Devens, Bruce H.
PATENT ASSIGNEE(S): Syntex (U.S.A.), Inc., USA
SOURCE: U.S., 15 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5001124	A	19910319	US 1990-474430	19900202
US 5108999	A	19920428	US 1990-631181	19901219
CA 2035544	AA	19910803	CA 1991-2035544	19910201
FI 9100503	A	19910803	FI 1991-503	19910201
NO 9100395	A	19910805	NO 1991-395	19910201
EP 440503	A1	19910807	EP 1991-300837	19910201
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
AU 9170165	A1	19910808	AU 1991-70165	19910201
AU 643494	B2	19931118		
HU 60479	A2	19920928	HU 1991-354	19910201
ZA 9100782	A	19921028	ZA 1991-782	19910201
JP 06340641	A2	19941213	JP 1991-216687	19910201
US 5328907	A	19940712	US 1992-818185	19920108
PRIORITY APPLN. INFO.:			US 1990-474430 A3	19900202
			US 1990-631181 A3	19901219

OTHER SOURCE(S): MARPAT 115:159126
GI



I



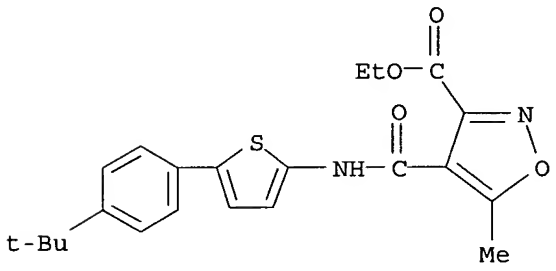
II

AB The title compds. [I; R1 = OH, PhO, (un)substituted alkoxy, etc.; R2 = (phenyl)alkyl, Ph; R3 = halo, OH, alkyl, haloalkoxy, etc.; Z = bond, 2,5-thienylenediyl, 2,5-furanylenediyl] were prepared as antiinflammatories and immunomodulators (no data). Thus, diketene was condensed with 4-(F3C)C6H4NH2 and the product condensed with pyrrolidine to give MeCR:CH2CONHC6H4CF3-4 (R = pyrrolidino) which was cyclocondensed with EtO2CC(Cl):NOH to give title compound II.

IT **134889-18-2P 134889-19-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as antiinflammatory and immunomodulator)

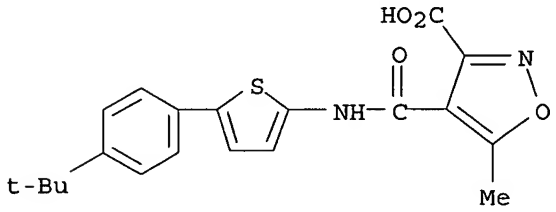
RN 134889-18-2 CAPLUS

CN 3-Isoxazolecarboxylic acid, 4-[[[5-[4-(1,1-dimethylethyl)phenyl]-2-thienyl]amino]carbonyl]-5-methyl-, ethyl ester (9CI) (CA INDEX NAME)



RN 134889-19-3 CAPLUS

CN 3-Isoxazolecarboxylic acid, 4-[[[5-[4-(1,1-dimethylethyl)phenyl]-2-thienyl]amino]carbonyl]-5-methyl- (9CI) (CA INDEX NAME)



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